Topics in shape-constrained inference

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This dissertation is submitted for the degree of
Doctor of Philosophy

Trinity College

October 2020

Declaration

This thesis is the result of my own work and includes nothing which is the outcome of work done in collaboration except as declared in the Preface and specified in the text. It is not substantially the same as any that I have submitted, or, is being concurrently submitted for a degree or diploma or other qualification at the University of Cambridge or any other University or similar institution except as declared in the Preface and specified in the text. I further state that no substantial part of my thesis has already been submitted, or, is being concurrently submitted for any such degree, diploma or other qualification at the University of Cambridge or any other University or similar institution except as declared in the Preface and specified in the text. It does not exceed the prescribed word limit for the relevant Degree Committee.

Chapter 2 is joint work with Adityanand Guntuboyina (University of California Berkeley), Arlene Kim (Korea University) and Richard Samworth (University of Cambridge), and has been published in the *Annals of Statistics* as Feng et al. (2021a). Chapter 3 is joint work with Yining Chen (London School of Economics), Qiyang Han (Rutgers University), Raymond Carroll (Texas A&M University) and Richard Samworth (University of Cambridge), and has been submitted for publication as Feng et al. (2021b).

Oliver Yuanhong Feng
October 2020

Acknowledgements

First and foremost, I would like to express my sincere gratitude to my supervisor Professor Richard Samworth for his support and guidance over the last few years. As an undergraduate, I was fortunate to have had the opportunity to do two summer projects and a Part III essay with him, which whetted my appetite for Statistics and persuaded me to pursue a PhD in the area. It has been a real privilege to work closely with him on a number of projects, and I have learned a great deal in the process. He has been extremely generous with his time, and his careful advice and feedback have been invaluable.

I have also benefitted hugely from my involvement in Richard's research group, not least because of the breadth of expertise and the positive atmosphere within it. For being a constant source of inspiration and encouragement, I would like to thank Tom Berrett, Tim Cannings, Yudong Chen, Milana Gataric, Jana Janková, Anton Lundborg, Philip Thompson, Tengyao Wang, Min Xu, Yi Yu, Yoav Zemel and Ziwei Zhu.

It is a pleasure to have the opportunity to thank my collaborators Ray Carroll, Yining Chen, Aditya Guntuboyina, Qiyang Han, Arlene Kim, Cindy Rush and Ramji Venkataramanan for their many helpful insights and suggestions during our regular Skype meetings, sometimes at ungodly hours in their parts of the world.

Thanks also to my examiners Richard Nickl and Yannick Baraud for their careful reading of this thesis, and for a useful and stimulating discussion.

Back in the days when international travel was still possible, I enjoyed a month-long visit to the University of Chicago hosted by Rina Foygel Barber, whose generosity and hospitality I very much appreciated. It was lovely to spend time with Ran Dai, Haoyang Liu, Antoine Picard and Fan Yang during my stay.

I am indebted to many other friends and colleagues in the CMS for their warmth and good humour, including Benjamin Barrett, Lawrence Barrott, Michal Buran, Nigel Burke, Alex Chamolly, Derek Driggs, Nicolas Dupré, Tom Edinburgh, Jo Evans, Tamara Großmann, Adam P. Goucher, James Kilbane, James Munro, Florian Pein, Sam Power, Torben Sell, Ferdia Sherry, Benjamin Stokell, Rita Teixeira da Costa, Sam Thomas and Sven Wang.

Finally, I would like to thank my family for their unstinting love and support, especially during the past year. Their strength and resilience have been an inspiration to me.

Abstract

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This thesis consists of three chapters. In the introductory Chapter 1, we survey the field of nonparametric inference under shape constraints, focussing in particular on the topics of shape-restricted regression and shape-constrained density estimation.

In Chapter 2, we investigate the adaptation properties of the log-concave maximum likelihood estimator $\hat{f}_n$ of a multivariate log-concave density f_0. Our main theoretical results demonstrate that in certain situations where the true density f_0 has additional structure, the estimator $\hat{f}_n$ can attain rates of convergence (with respect to squared Hellinger distance or Kullback–Leibler divergence) that are strictly faster than the global minimax convergence rate. We illustrate three different types of adaptive behaviour in dimensions $d = 2, 3$ through sharp oracle inequalities, which reveal that:

(i) $\hat{f}_n$ achieves essentially parametric rates of convergence when f_0 is close to a log-concave density with polyhedral support whose logarithm is piecewise affine;

(ii) $\hat{f}_n$ attains the rate $n^{-4/(d+4)}$ up to logarithmic factors when $d = 3$ and f_0 is well-approximated by a log-concave density that is bounded away from zero on a polytopal support;

(iii) $\hat{f}_n$ satisfies an adaptive risk bound of order $n^{-\min\left(\frac{\beta+3}{\beta+7}, \frac{4}{7}\right)}$ when $d = 3$ and f_0 is close to a log-concave density that is β-Hölder for $\beta > 1$ (and more generally when the approximating density satisfies a novel 'contour separation' condition).

Our approach entails developing local bracketing entropy bounds for Hellinger neighbourhoods of log-concave densities that belong to the special subclasses described above. To this end, we apply techniques from convex geometry and real analysis to elucidate the structural properties of such densities, and obtain some results of independent interest.

In Chapter 3, we consider the nonparametric estimation of an S-shaped regression function. The least squares estimator provides a very natural, tuning-free approach, but results in a non-convex optimisation problem, since the inflection point is unknown. We show that the estimator may nevertheless be regarded as a projection onto a finite union of convex cones, which allows us to propose a mixed primal-dual bases algorithm for its efficient, sequential computation. After developing a general projection framework that demonstrates the consistency and robustness to misspecification of the estimator, we prove worst-case and adaptive risk bounds for the estimation of the regression function, in the form of sharp oracle inequalities, and establish bounds on the rate of convergence of the estimated inflection point. These theoretical results reveal not only that the estimator achieves the minimax optimal rate for both the estimation of the regression function and its inflection point (up to a logarithmic factor in the latter case), but also that it is able to achieve an almost-parametric rate when the true regression function is piecewise affine with not too many affine pieces. Simulations also confirm the desirable finite-sample properties of the estimator, and our algorithm is implemented in the `R` package `Sshaped`.

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Chapter 1

Introduction

This thesis is a contribution to the considerable and growing literature on the development and analysis of shape-constrained methods for statistical inference. Broadly speaking, these seek to avoid imposing restrictive parametric assumptions on an unknown function of interest by instead enforcing only a (global) shape restriction such as monotonicity, convexity or log-concavity. In many applications, this approach is often justifiable and even desirable in view of specific practical considerations. A hallmark of many shape-constrained procedures is that they can enjoy the best of the parametric and nonparametric worlds: as well as being flexible and versatile for modelling purposes, they often also have the virtue of being fully automatic in that they do not require the choice of one or more tuning parameters. This is in contrast to orthogonal series estimators and traditional nonparametric smoothing techniques based on splines or kernels (e.g. Giné and Nickl, 2016; Silverman, 1986; Wand and Jones, 1994, Chapter 5), for which tuning parameter (e.g. bandwidth) selection is a non-trivial task both in theory and in practice, particularly in multivariate settings.

Much of the early work on shape-constrained inference was centred around univariate order restrictions such as monotonicity and unimodality (Barlow et al., 1972; Robertson et al., 1988). The resulting methodological and computational frameworks were found to have wide applicability in a variety of statistical contexts, including but not limited to regression, density estimation, interval censoring models, survival analysis and deconvolution problems. An initial challenge for theoreticians was to elucidate the unusual asymptotic behaviour of univariate monotonicity-constrained estimators, notably their cube-root rates of convergence and non-standard pointwise limiting distributions (Groeneboom, 1985; Prakasa Rao, 1969). This asymptotic theory was later extended to convexity-constrained models and applied in the construction of pointwise confidence intervals for local parameters (e.g. Balabdaoui, Rufibach and Wellner, 2009; Banerjee and Wellner, 2001; Deng et al., 2021; Groeneboom et al., 2001). For a comprehensive account of the topics mentioned thus far, see Groeneboom and Jongbloed (2014).

In the 21st century, research activity in the field of shape constraints has significantly intensified and diversified, as has been documented in a 2018 special issue of *Statistical Science*. The area has been enriched by methodological innovations in new directions, including log-concave density estimation (Cule et al., 2010; Dümbgen and Rufibach, 2009; Dümbgen et al., 2011), convex set estimation (Brunel, 2013; Gardner et al., 2006; Guntuboyina, 2012), shape-constrained dimension reduction (Chen and Samworth, 2016; Groeneboom and Hendrickx, 2018; Xu et al., 2016), and ranking and pairwise or multiway comparisons (Pananjady and Samworth, 2020; Shah et al., 2017). To maximise the impact of these developments on statistical practice, an ongoing line of work aims to devise and implement new algorithms for some shape-constrained problems that were previously intractable for large or high-dimensional datasets (Chen and Mazumder, 2020; Koenker and Mizera, 2014; Mazumder et al., 2018). This has already attracted some interest from the theoretical computer science community (e.g. Axelrod et al., 2019), and in the years to come, it is likely that insights and practical motivation from other disciplines will lead to further advances.

On the theoretical front, new tools developed recently (Bellec, 2018; Cai and Low, 2015; Chatterjee, 2014; Dümbgen et al., 2011; Guntuboyina and Sen, 2013; Han, 2021) have enabled us to discover many more intriguing properties of shape-constrained estimators. In the past decade or so, the overall emphasis has shifted away from univariate asymptotic results and more towards finite-sample analysis with respect to global loss functions in general dimensions. Minimax rates of convergence* are now known for a variety of shape-constrained estimation problems, including decreasing density estimation on the non-negative half-line (Birgé, 1987), isotonic regression (Chatterjee et al., 2018; Deng and Zhang, 2020; Han et al., 2019; Zhang, 2002), convex regression (Han and Wellner, 2016a; Kur et al., 2020) and log-concave density estimation (Kim and Samworth, 2016; Kur et al., 2019). In particular, some of these recent works have shed light on interesting and often surprising multivariate phenomena in different contexts, and efforts are being made to explain these findings in a unified way (Han, 2021).

In the rest of this Introduction, we will provide a more detailed summary of the general paradigms, core problems and major achievements of the field of nonparametric shape-constrained inference, with a focus on the twin pillars of regression and density estimation. In doing so, we will introduce some key themes that will be developed further in the rest of the thesis. Prominent among these is the important topic of *adaptation*. Even though this has been studied extensively in the literature on general nonparametric function estimation (e.g. Giné and Nickl, 2016, Chapter 8), it is only recently that sustained progress has been made in understanding the global adaptive behaviour of tuning-free shape-constrained estimators. A particularly effective way of illustrating rate adaptation in finite samples is through (sharp) *oracle inequalities*, since these also provide tight control on the deterioration in statistical performance that may occur when the unknown true function deviates from an assumed model or submodel. In other words, they provide guarantees on the robustness of estimation procedures under forms of model misspecification, which are highly sought after in modern statistics.

1.1 Shape-restricted regression and constrained least squares estimators

A generic nonparametric regression model takes the form

$$Y_i = f_0(X_i) + \xi_i, \quad i = 1, \dots, n, \tag{1.1.1}$$

where $Y_1, \dots, Y_n$ are real-valued observations, $f_0 \colon \mathcal{X} \to \mathbb{R}$ is an unknown regression function defined on some covariate domain $\mathcal{X}$ (typically a subset of $\mathbb{R}^d$ for some $d \in \mathbb{N}$), $X_1, \dots, X_n$ are fixed or random design points taking values in $\mathcal{X}$, and $\xi_1, \dots, \xi_n$ are unobserved mean-zero errors (with finite variances) that are independent of $X_1, \dots, X_n$.

A statistical inference problem in this setting is to find an appropriate *estimator* of f_0 based on $(X_1, Y_1), \dots, (X_n, Y_n)$, that is to say a function $\tilde{f}_n \colon \mathcal{X} \to \mathbb{R}$ that depends measurably on $\{(X_i, Y_i) : 1 \le i \le n\}$. To make precise what we mean by an 'appropriate' or 'good' estimator $\tilde{f}_n$, we need to introduce a loss function L to measure the deviation of $\tilde{f}_n$ from the true f_0. A common choice is $L(\tilde{f}_n, f_0) = \|\tilde{f}_n - f_0\|^2_{L^2(\mathbb{P}_n^X)} := n^{-1} \sum_{i=1}^n \bigl(\tilde{f}_n(X_i) - f_0(X_i)\bigr)^2$, which only takes into account the errors incurred at the design points, while for random designs where $X_1, \dots, X_n \overset{\mathrm{iid}}{\sim} P^X$ for some

*In the interests of transparency, we note that in some of our examples, there remain gaps between the known minimax lower and upper bounds that are polylogarithmic in the sample size.

distribution P^X on $\mathcal{X}$, another option is $L(\tilde{f}_n, f_0) = \|\tilde{f}_n - f_0\|^2_{L^2(P^X)} := \int_{\mathcal{X}} (\tilde{f}_n - f_0)^2 \, dP^X$. The performance of an estimator $\tilde{f}_n$ can then be quantified through its risk $R(\tilde{f}_n, f_0) := \mathbb{E}\bigl(L(\tilde{f}_n, f_0)\bigr)$ with respect to L under (1.1.1).

Turning now to shape-restricted regression (cf. Guntuboyina and Sen, 2018), suppose we have reason to believe that the true f_0 satisfies a global shape constraint such as convexity or some form of monotonicity. Writing $\tilde{\mathcal{F}}$ for the class of all candidate functions with this property, we say that $\hat{f}_n$ is a *least squares estimator* over $\tilde{\mathcal{F}}$ based on $\{(X_i, Y_i) : 1 \leq i \leq n\}$ if $\hat{f}_n \in \operatorname{argmin}_{f \in \tilde{\mathcal{F}}} \sum_{i=1}^n \bigl(Y_i - f(X_i)\bigr)^2$, so that $\hat{f}_n$ is an empirical risk minimiser. Even when least squares estimators exist, the best we can hope for in terms of uniqueness is that they are well defined on $\{X_1, \ldots, X_n\}$, for example when $\tilde{\mathcal{F}}$ is closed and convex. In these cases, we often extend the fitted values to the whole of $\mathcal{X}$ in a manner consistent with the shape constraint on $\tilde{\mathcal{F}}$ (e.g. in a piecewise constant or piecewise affine fashion), thus yielding a concretely defined $\hat{f}_n$ that we can refer to as *the* least squares estimator over $\tilde{\mathcal{F}}$. We also remark that when $\tilde{\mathcal{F}}$ is a shape-constrained class, least squares estimators $\hat{f}_n$ generally do not interpolate the data $\{(X_i, Y_i) : 1 \leq i \leq n\}$ exactly.

In the rest of this section, we will mostly restrict attention to fixed design settings where $X_i \equiv x_i \in \mathcal{X}$ for $1 \leq i \leq n$, although we will briefly comment on random designs where appropriate. Writing $\theta_0 := \bigl(f_0(x_1), \ldots, f_0(x_n)\bigr)$, $Y := (Y_1, \ldots, Y_n)$ and $\xi := (\xi_1, \ldots, \xi_n)$, we can rewrite (1.1.1) in the form

$$Y = \theta_0 + \xi \tag{1.1.2}$$

when the design points $x_1, \ldots, x_n \in \mathcal{X}$ are fixed. In this case, let

$$\Theta \equiv \Theta(\tilde{\mathcal{F}}) := \bigl\{\bigl(f(x_1), \ldots, f(x_n)\bigr) : f \in \tilde{\mathcal{F}}\bigr\} \tag{1.1.3}$$

and define $\hat{\theta}_n$ to be a least squares estimator of θ_0 over Θ if $\hat{\theta}_n \in \operatorname{argmin}_{\theta \in \Theta} \|Y - \theta\|^2$, where $\|u\|^2 := \sum_{i=1}^n u_i^2$ for $u \equiv (u_1, \ldots, u_n) \in \mathbb{R}^n$, so that $\hat{\theta}_n = \bigl(\hat{f}_n(x_1), \ldots, \hat{f}_n(x_n)\bigr)$ for some least squares estimator $\hat{f}_n$ over $\tilde{\mathcal{F}}$. The risk of $\hat{\theta}_n$ is then given by

$$R(\hat{\theta}_n, \theta_0) := \mathbb{E}(\|\hat{\theta}_n - \theta_0\|^2/n) = \mathbb{E}\bigl(\|\hat{f}_n - f_0\|^2_{L^2(\mathbb{P}_n^X)}\bigr)$$

under (1.1.2). If Θ is closed, then $\hat{\theta}_n$ exists, and if in addition Θ is convex, then $\hat{\theta}_n$ is unique and coincides with the unique *projection* of Y onto Θ. For the shape-constrained classes $\tilde{\mathcal{F}}$ we exhibit below (and in the rest of the thesis), the associated $\Theta(\tilde{\mathcal{F}})$ is either a closed, convex cone or a finite union of closed, convex cones.

Before discussing any specific shape constraints, we first outline some general approaches for deriving bounds on the finite-sample risk $R(\hat{\theta}_n, \theta_0)$ for constrained least squares estimators over closed, convex sets Θ, at least when the noise variables are independent and (sub)-Gaussian. It turns out that $R(\hat{\theta}_n, \theta_0)$ is intimately connected with certain complexity measures for closed, convex sets Θ. The first of these is the *localised Gaussian width*

$$w_{\theta_0}(t; \Theta) := \mathbb{E}\biggl(\sup_{v \in \Theta : \|v - \theta_0\| \leq t} Z^\top (v - \theta_0)\biggr), \tag{1.1.4}$$

where $Z \sim N_n(0, I_n)$ and $t \geq t_{\min} := \inf_{\theta \in \Theta} \|\theta - \theta_0\|$; note that the signal $\theta_0 \in \mathbb{R}^n$ in (1.1.2) is not required to belong to Θ. A remarkable result of Chatterjee (2014) asserts that the function $t \mapsto w_{\theta_0}(t; \Theta) - t^2/2$ has a unique maximiser t_{θ_0} in $[t_{\min}, \infty)$, and that if $\xi \sim N_n(0, I_n)$ in (1.1.1), then the random quantity $\|\hat{\theta}_n - \theta_0\|$ concentrates around t_{θ_0}, with fluctuations of order $\sqrt{t_{\theta_0}}$. In fact, an exponential tail bound holds for $\|\hat{\theta}_n - \theta_0\| - t_{\theta_0}$, which implies in particular that

$$|R(\hat{\theta}_n, \theta_0) - t_{\theta_0}^2| \leq C\bigl(t_{\theta_0}^{3/2} \vee 1\bigr).$$

Consequently, the task of establishing upper and lower bounds on $R(\hat{\theta}_n, \theta_0)$ for specific regression models (1.1.2) can be reduced to that of bounding $w_{\theta_0}(t;\Theta)$ in (1.1.4). One way to do this is through metric entropy bounds for Θ and Dudley's entropy integral, which is used to control the expected suprema of Gaussian processes via a chaining argument (e.g. Giné and Nickl, 2016, Chapter 2.3).

Another elegant and powerful device is based on the notion of *statistical dimension* (Amelunxen et al., 2014), which for a closed, convex cone $\Lambda \subseteq \mathbb{R}^n$ is defined as

$$\delta(\Lambda) := \mathbb{E}\biggl\{\biggl(\sup_{v\in\Lambda:\|v\|\leq 1} Z^\top v\biggr)^2\biggr\}, \tag{1.1.5}$$

where $Z \sim N_n(0, I_n)$ as above. It can in fact be shown that $\delta(\Lambda) = \mathbb{E}(\|\Pi_\Lambda(Z)\|^2)$, where $\Pi_\Lambda \colon \mathbb{R}^n \to \Lambda$ denotes the projection onto Λ, and hence that this coincides with the usual concept of dimension when Λ is a linear subspace. Now for a closed, convex set Θ and $\theta \in \Theta$, the *tangent cone* $T_\Theta(\theta)$ of Θ at θ is defined as the closure of $\{\lambda(v-\theta) : v \in \Theta,\ \lambda \geq 0\}$, and under (1.1.2), an important 'basic inequality' (Bellec, 2018, Proposition 2.1) is that

$$\|\hat{\theta}_n - \theta_0\|^2 \leq \inf_{\theta\in\Theta} \bigl\{\|\theta - \theta_0\|^2 + \|\Pi_{T_\Theta(\theta)}(\xi)\|^2\bigr\}. \tag{1.1.6}$$

This holds for all $\theta_0 \in \mathbb{R}^n$ as above, not just those in Θ, and since this is a consequence of a deterministic result, no distributional assumptions on ξ are needed. That said, when $\xi \sim N_n(0, I_n)$, it follows from (1.1.5) and (1.1.6) that

$$R(\hat{\theta}_n, \theta_0) \leq \frac{1}{n} \inf_{\theta\in\Theta} \bigl\{\|\theta - \theta_0\|^2 + \delta\bigl(T_\Theta(\theta)\bigr)\bigr\}, \tag{1.1.7}$$

and a exponential tail bound for $\|\hat{\theta}_n - \theta_0\|^2$ can also be obtained. The risk bound (1.1.7) is an example of a *sharp oracle inequality*, in which $\|\theta - \theta_0\|^2/n$ is an approximation error term that quantifies the effect of model misspecification (since θ_0 need not belong to Θ). The 'sharpness' here refers to the fact that this term has leading constant 1 on the right hand side. We remark that (1.1.7) can be extended to regression models where $\xi_1, \ldots, \xi_n$ are independent, sub-Gaussian random variables with parameter 1, and that slighter weaker analogues hold when Θ is a closed, non-convex set (e.g. when Θ is a finite union of closed, convex cones). A different method for obtaining oracle inequalities is again based on localised Gaussian widths (1.1.4) and the function $t \mapsto w_{\theta_0}(t;\Theta) - t^2/2$ (Bellec, 2018, Section 2.2), although this is somewhat different in flavour from the approach of Chatterjee (2014).

To develop the bound (1.1.7) for specific constrained least squares estimators, we need to be able to control the statistical dimensions of tangent cones of Θ. For this purpose, it is often helpful to make use of some convenient properties of the statistical dimension; for example, if $\Lambda \subseteq \Lambda' \subseteq \mathbb{R}^n$ are nested closed, convex cones, then $\delta(\Lambda) \leq \delta(\Lambda')$, and if Λ_1, Λ_2 are closed, convex cones in $\mathbb{R}^{n_1}, \mathbb{R}^{n_2}$ respectively, then $\Lambda_1 \times \Lambda_2$ is a closed, convex cone in $\mathbb{R}^{n_1+n_2}$ with $\delta(\Lambda_1 \times \Lambda_2) = \delta(\Lambda_1) + \delta(\Lambda_2)$ (Amelunxen et al., 2014, Proposition 3.1). It turns out that in the univariate isotonic regression problem that we go on to describe, there is an exact expression (Amelunxen et al., 2014; Soloff et al., 2019) for the statistical dimension of the monotone cone $\Theta^\uparrow$ in (1.1.9), namely

$$\delta(\Theta^\uparrow) = \sum_{j=1}^{n} \frac{1}{j}. \tag{1.1.8}$$

This yields the adaptive risk bound (1.3.1) that we discuss in Section 1.3.

1.1.1 Isotonic regression and order restrictions

As mentioned previously, there is a large body of work on inference under monotonicity constraints, dating back as far as Ayer et al. (1955), Brunk (1955) and van Eeden (1956). In univariate isotonic regression, we work with the class $\tilde{\mathcal{F}} = \mathcal{F}^{\uparrow}$ of non-decreasing functions $f\colon \mathbb{R} \to \mathbb{R}$ and take the least squares estimator $\hat{f}_n$ over $\mathcal{F}^{\uparrow}$ to be a left-continuous, piecewise constant function, with jumps only at design points. Under the model (1.1.1), observe that in both fixed and random designs, the quantity $\mathbb{E}\bigl(\|\hat{f}_n - f_0\|^2_{L^2(\mathbb{P}_n^X)}\big|X_1,\dots,X_n\bigr)$ depends on $X_1,\dots,X_n$ only through $\{f_0(X_i) : 1 \leq i \leq n\}$ and the ordering of $X_1,\dots,X_n$ on the real line. When $x_1 < \cdots < x_n$ are fixed design points, the constraint set (1.1.3) for the model (1.1.2) is the monotone cone

$$\Theta^{\uparrow} := \{\theta \equiv (\theta_1,\dots,\theta_n) \in \mathbb{R}^n : \theta_1 \leq \cdots \leq \theta_n\}. \tag{1.1.9}$$

Basic properties and computation: In contrast to most other shape-constrained estimators, the isotonic least squares estimator $\hat{\theta}_n \equiv (\hat{\theta}_{n1},\dots,\hat{\theta}_{nn}) = \operatorname{argmin}_{\theta\in\Theta^{\uparrow}} \|Y - \theta\|$ over $\Theta^{\uparrow}$ can be explicitly characterised. One useful identity is the *min-max formula* $\hat{\theta}_{ni} = \min_{b\geq i}\max_{a\leq i}\sum_{j=a}^{b} Y_j/(b-a+1)$ for $1 \leq i \leq n$. An alternative representation is in terms of the left derivative of the greatest convex minorant of the cumulative sum diagram associated with $\{Y_i : 1 \leq i \leq n\}$, as formalised below.

Proposition 1.1.1 (e.g. Groeneboom and Jongbloed, 2018, Lemma 2.1)**.** *Let $\hat{F}_n$ be the greatest convex function on $[0,1]$ satisfying $\hat{F}_n(0) \leq 0$ and $\hat{F}_n(i/n) \leq \sum_{j=1}^{i} Y_j/n$ for all $1 \leq i \leq n$. Then writing $\hat{F}_n'(x)$ for the left derivative of $\hat{F}_n$ at $x \in (0,1]$, we have $\hat{\theta}_{ni} = \hat{F}_n'(i/n)$ for all $1 \leq i \leq n$.*

It can be seen that $\hat{\theta}_n \equiv (\hat{\theta}_{n1},\dots,\hat{\theta}_{nn})$ is a piecewise constant, non-decreasing sequence such that on each constant piece, the common value is the average of the corresponding observations Y_i in the block. Based on Proposition 1.1.1, the isotonic least squares estimator $\hat{\theta}_n$ can be computed efficiently using the 'pool adjacent violators' algorithm (PAVA), which has $O(n)$ complexity in time and space. This sweeps from left to right and always ensures that a correctly ordered block structure is maintained before it adds the next observation Y_i to the right. If this results in a violation of monotonicity, the new singleton block is merged with the block immediately to the left, and the appropriate weighted average is then assigned to the combined block. This process of block amalgamation is iterated until the entire sequence is once again non-decreasing. In Sections 3.2 and 3.5.2, we will present a generalisation of PAVA for convex least squares problems that is also based on a sequential computational strategy.

Univariate asymptotic theory: As mentioned previously, isotonic least squares estimators exhibit non-standard pointwise asymptotics. Assume for simplicity that $x_i = i/n$ for $1 \leq i \leq n$, so that $\hat{f}_n(i/n) = \hat{\theta}_{ni} = \hat{F}_n'(i/n)$ for $1 \leq i \leq n$, and suppose that the errors $\xi_1,\dots,\xi_n$ in (1.1.1) are i.i.d. with mean zero and variance 1. It was shown by Brunk (1970), among others, that if the true regression function $f_0 \in \mathcal{F}^{\uparrow}$ and $t \in (0,1)$ are such that f_0 has a positive continuous derivative on a neighbourhood of t, then

$$n^{1/3}\bigl(\hat{f}_n(t) - f_0(t)\bigr) \xrightarrow{d} \bigl(4f_0'(t)\bigr)^{1/3}\,\mathcal{L}, \tag{1.1.10}$$

where $\mathcal{L}$ denotes the Chernoff distribution (Groeneboom and Jongbloed, 2014, Section 3.9). Since $f_0'(t)$ is unknown and is not straightforward to estimate, (1.1.10) cannot be used directly to construct asymptotically valid confidence intervals for $f_0(t)$. An asymptotically pivotal quantity for this problem has recently been obtained by Deng et al. (2021). Other useful techniques include bootstrap resampling methods and likelihood ratio tests (Banerjee and Wellner, 2001).

Univariate non-asymptotic results: Zhang (2002) showed using martingale methods that in correctly specified models (1.1.2) where $\theta_0 \equiv (\theta_{01},\dots,\theta_{0n}) \in \Theta^{\uparrow}$ and $\xi_1,\dots,\xi_n$ are i.i.d. with mean zero and variance 1, there is a universal constant $C > 0$ such that

$$R(\hat{\theta}_n, \theta_0) \leq C\left\{\left(\frac{\theta_{0n} - \theta_{01}}{n}\right)^{2/3} + \frac{\log(en)}{n}\right\}. \tag{1.1.11}$$

It follows from this and a complementary local minimax lower bound (Chatterjee et al., 2015, Theorem 5.3) that $\hat{\theta}_n$ attains the minimax rate over the classes $\{\theta_0 \in \Theta^{\uparrow} : \theta_{0n} - \theta_{01} \leq V\}$ for $n^{-1/2} \lesssim V \lesssim n^{1/2}$. When $\xi_1, \ldots, \xi_n$ are independent sub-Gaussian random variables with parameter 1, (1.1.11) can be extended to a sharp oracle inequality for general $\theta_0 \in \mathbb{R}^n$ (Bellec, 2018, Corollary 3.3), similar to (1.1.14) below.

Other interesting recent works on univariate isotonic regression include Yang and Barber (2019), which exploits properties of the projection onto the monotone cone $\Theta^{\uparrow}$ to derive confidence bands for an isotonic signal $\theta_0 \in \Theta^{\uparrow}$, and Dai et al. (2020), which studies the bias of $\hat{\theta}_{ni}$ as an estimator of θ_{0i} for $1 \leq i \leq n$ (under 'smoothness conditions' on θ_0).

Multivariate extensions: In the last few years, progress has also been made on multivariate isotonic regression problems involving more general order restrictions. When the covariate domain $\mathcal{X}$ in (1.1.1) is taken to be $[0,1]^d$ for some general $d \in \mathbb{N}$, a natural analogue of the class $\mathcal{F}^{\uparrow}$ of non-decreasing functions on $\mathbb{R}$ is the set $\mathcal{F}_d^{\uparrow}$ of all block-increasing functions $f\colon [0,1]^d \to \mathbb{R}$ satisfying $f(x) \leq f(x')$ whenever $x_j \leq x_j'$ for all $1 \leq j \leq d$. More generally, for a directed graph $G = (V, E)$ with vertex set V and edge set E, we can define a relation $\preceq$ on V by setting $v \preceq v'$ if there is a directed path from v to v' in G, and then take $\mathcal{F}^{\uparrow}(G)$ to be the set of $f\colon V \to \mathbb{R}$ such that $f(v) \leq f(v')$ whenever $v \preceq v'$. Since $\preceq$ is usually not a total order, many insights from the original univariate setting do not generalise straightforwardly, although there is a version of the min-max formula for least squares estimators over $\mathcal{F}^{\uparrow}(G)$.

In isotonic regression problems featuring $\mathcal{F}_d^{\uparrow}$ in dimensions $d \geq 2$, results for the fixed design setting have mainly focussed on cubic lattice designs $\mathbb{L}_{d,n}$ (aligned with the coordinate axes). Writing $\Theta^{\uparrow}(\mathbb{L}_{d,n}) \subseteq \mathbb{R}^n$ for the induced constraint set (1.1.3) and $B_\infty(1)$ for the set of $\theta_0 \in \mathbb{R}^n$ with uniform norm bounded by 1, we now know that the least squares estimator $\hat{\theta}_n$ over $\Theta^{\uparrow}(\mathbb{L}_{d,n})$ satisfies

$$\sup_{\theta_0 \in \Theta^{\uparrow}(\mathbb{L}_{d,n}) \cap B_\infty(1)} R(\hat{\theta}_n, \theta_0) \lesssim n^{-1/d} \log^{5/2} n$$

when $\xi_1, \ldots, \xi_n \overset{\mathrm{iid}}{\sim} N(0,1)$; see Pananjady and Samworth (2020, Corollary 1(b)), which improves the polylogarithmic factor in Han et al. (2019, Theorem 1). The minimax rate over $\Theta^{\uparrow}(\mathbb{L}_{d,n}) \cap B_\infty(1)$ has been shown to be of order $n^{-1/d}$, and this is attained (up to a multiplicative factor depending only on d) by a 'block-isotonic' estimator based on a min-max formula (Deng and Zhang, 2020).

It is somewhat surprising that the isotonic least squares estimator is essentially minimax rate optimal when $d \geq 3$, given the complexity of the underlying function class (comprising those $f \in \mathcal{F}_d^{\uparrow}$ with uniform norm at most 1). Indeed, it was previously believed that in these dimensions, the rapid divergence of the associated entropy integral ought to preclude rate optimality for empirical risk minimisation procedures (Birgé and Massart, 1993; van de Geer, 2000). This phenomenon has been studied from a more general perspective by Han (2021), who demonstrates in particular that the behaviour of the least squares estimator is governed by the complexity of a class of upper and lower *sets* in $[0,1]^d$.

Thus far, we have only covered aspects of the *worst-case* performance of isotonic regression estimators. There is also an interesting *adaptation* story to tell, which we defer to Section 1.3. It is worth mentioning that Han et al. (2019) established worst-case and adaptive risk bounds of a similar flavour in the more challenging random design setting where $X_1, \ldots, X_n \overset{\mathrm{iid}}{\sim} P$, for some distribution

P on $[0,1]^d$ with a Lebesgue density bounded away from 0 and ∞. Deng and Zhang (2020) have also obtained results for block estimators in isotonic regression on general directed graphs.

To conclude our discussion of isotonic regression for the time being, we remark that little is known about the pointwise asymptotic behaviour of least squares estimators in general dimensions, although Deng et al. (2021) have recently shown that pivotal limiting distributions based on block-isotonic estimators can be used to construct pointwise confidence intervals. Also, there has been another line of work on 'uncoupled' isotonic regression problems where it is not completely known to which design point X_i each observation Y_i corresponds (e.g. Carpentier and Schlueter, 2016; Mao et al., 2020; Pananjady and Samworth, 2020; Rigollet and Weed, 2019).

1.1.2 Convex regression

Convexity is another natural restriction to impose on a regression function, for example in the context of production and utility curves in economics (e.g. Hildreth, 1954; Matzkin, 1991; Varian, 1984). In the univariate setting where $\mathcal{X} = [0,1]$ is the covariate domain and $\mathcal{C}$ denotes the class of all convex $f\colon [0,1] \to \mathbb{R}$, the least squares estimator $\hat{f}_n$ over $\mathcal{C}$ is taken to be a piecewise affine function with knots only at design points. While it has an implicit characterisation in terms of the optimality conditions for the constrained least squares problem (Groeneboom et al., 2001, Lemma 2.6), there is no explicit representation analogous to Proposition 1.1.1. Observe that in fixed design settings where $x_1 < \cdots < x_n$, the constraint set

$$\Theta(\mathcal{C}) = \left\{(\theta_1, \ldots, \theta_n) \in \mathbb{R}^n : \frac{\theta_2 - \theta_1}{x_2 - x_1} \leq \cdots \leq \frac{\theta_n - \theta_{n-1}}{x_n - x_{n-1}}\right\}$$

is a closed, convex cone that now depends on the design points through their (relative) spacings. In most of the theoretical work on this topic, it has typically been assumed that these points are equispaced, 'near-equispaced' or 'well-separated' in a suitable sense.

Univariate asymptotic theory: For example, pointwise asymptotic results have been derived for triangular array schemes where for each n, the design points $x_i \equiv x_{ni}$ satisfy $c/n \leq x_i - x_{i-1} \leq C/n$ for $2 \leq i \leq n$ and universal constants $0 < c < C$, and the errors $\xi_i \equiv \xi_{ni}$ are i.i.d. subexponential random variables with parameter 1. In this setup, when the true regression function $f_0\colon [0,1] \to \mathbb{R}$ is convex, and $x_0 \in (0,1)$ is such that $f_0''(x_0) > 0$ and f_0'' is continuous on a neighbourhood of x_0, Mammen (1991) showed that $\hat{f}_n(x_0)$ is $n^{2/5}$-consistent for estimating $f_0(x_0)$. Following on from this, Groeneboom et al. (2001) established the precise form of the non-degenerate limiting distribution of

$$\begin{pmatrix} n^{2/5}\bigl(\hat{f}_n(x_0) - f_0(x_0)\bigr) \\ n^{1/5}\bigl(\hat{f}_n'(x_0) - f_0'(x_0)\bigr) \end{pmatrix} \tag{1.1.12}$$

under an additional regularity condition. Results for different local smoothness regimes and the random design setting where $X_1, \ldots, X_n \overset{\text{iid}}{\sim} U[0,1]$ are also available (Chen and Wellner, 2016; Ghosal and Sen, 2017). Similarly to the isotonic case, (1.1.12) is not an asymptotically pivotal quantity since its limiting distribution depends on the nuisance parameter $f_0''(x_0)$. Instead, to obtain asymptotically valid pointwise confidence intervals for $f_0(x_0)$ and $f_0'(x_0)$, Deng et al. (2020) considered the kinks $\hat{v}_\pm(x_0)$ of $\hat{f}_n$ immediately to the left and right of x_0, and proved that

$$\begin{pmatrix} \sqrt{n\{\hat{v}_+(x_0) - \hat{v}_-(x_0)\}}\,\bigl(\hat{f}_n(x_0) - f_0(x_0)\bigr) \\ \sqrt{n\{\hat{v}_+(x_0) - \hat{v}_-(x_0)\}^3}\,\bigl(\hat{f}_n'(x_0) - f_0'(x_0)\bigr) \end{pmatrix} \tag{1.1.13}$$

has a universal limiting distribution under the same conditions as for (1.1.12).

Univariate risk bounds: For fixed designs, the first non-asymptotic results on the convex least squares estimator $\hat{\theta}_n$ over $\Theta(\mathcal{C})$ were again derived under the assumption that $c/n \leq x_i - x_{i-1} \leq C/n$ for $2 \leq i \leq n$. If in addition $\xi_1, \ldots, \xi_n$ are independent sub-Gaussian random variables with parameter 1, then for all signals $\theta_0 \equiv (\theta_{01}, \ldots, \theta_{0n}) \in \mathbb{R}^n$ in (1.1.2), there exists a universal constant $C' > 0$ such that

$$R(\hat{\theta}_n, \theta_0) \leq \inf_{\theta \in \Theta(\mathcal{C})} \left\{ \frac{1}{n}\|\theta - \theta_0\|^2 + \frac{C'\bigl(1 + V(\theta)\bigr)^{2/5}}{n^{4/5}} + \frac{4}{n} \right\},$$

where $V(\theta) := \max_{1 \leq i \leq n} \theta_i - \min_{1 \leq i \leq n} \theta_i$ for $\theta \in \mathbb{R}^n$. The proof of this sharp oracle inequality (Bellec, 2018, Corollary 4.4) is based on localised Gaussian width (1.1.4) and metric entropy considerations. See Guntuboyina and Sen (2015) and Chatterjee (2016) for similar results; a complementary local minimax lower bound of order $n^{-4/5}$ is also established in the former. The overall message here is that in convex regression with near-equispaced design points, the worst-case rate for the convex least squares estimator is faster than that of order $n^{-2/3}$ seen in isotonic or unimodal regression (Bellec, 2018, Appendix C). This is perhaps not unexpected given that convexity is a more restrictive constraint than unimodality.

When instead the design points are far from being equispaced, the worst-case behaviour of $\hat{\theta}_n$ can be very different. Under the same conditions on $\xi_1, \ldots, \xi_n$ as above, there exists a universal constant $C' > 0$ such that the sharp oracle inequality

$$R(\hat{\theta}_n, \theta_0) \leq \inf_{\theta \in \Theta(\mathcal{C})} \left\{ \frac{1}{n}\|\theta - \theta_0\|^2 + \frac{C'\bigl(1 + V(\theta)\bigr)^{2/3}}{n^{2/3}} + \frac{4}{n} \right\} \tag{1.1.14}$$

holds for all $\theta_0 \in \mathbb{R}^n$ and all configurations of design points $x_1 < \ldots < x_n$ (Bellec, 2018, Theorem 4.7). Furthermore, a minimax lower bound (Bellec, 2018, Theorem 4.5) shows that $\hat{\theta}_n$ actually attains the slower rate of order $n^{-2/3}$ in certain cases where the design points concentrate around the boundary of the covariate domain $[0, 1]$ and the successive gaps between them decay geometrically. In these situations, it would appear that the convexity constraint yields no gains in statistical performance over and above that which can be achieved under unimodality.

We mention in passing that in the random design setting where $X_1, \ldots, X_n \overset{\text{iid}}{\sim} P$ on $[0, 1]$, the $L^2(P)$ risk of the least squares estimator $\hat{f}_n$ can be infinite. This can happen even in seemingly non-pathological examples, such as when $P = U[0, 1]$, $f_0 \equiv 0$ and $Y_1, \ldots, Y_n \overset{\text{iid}}{\sim} U\{-1, 1\}$ (Balász et al., 2015). The reason for this is that $\hat{f}_n$ can blow up at the boundary of the covariate domain, where its behaviour is not tightly regulated by the global shape constraint. It is known for example that for $x \in \{0, 1\}$, the random variables $\hat{f}_n'(x)$ for $n \in \mathbb{N}$ are not bounded in probability, and that $\hat{f}_n(x)$ is not a consistent estimator of $f_0(x)$ (Ghosal and Sen, 2017, Lemma 5.1).

Multivariate convex regression — basic properties, computation and theory: For a general closed, convex covariate domain $\mathcal{X} \subseteq \mathbb{R}^d$ with $d \in \mathbb{N}$, the shape-constrained class is taken to be the set $\mathcal{C}(\mathcal{X})$ of all convex $f \colon \mathcal{X} \to \mathbb{R}$. By the convexity of $\mathcal{C}(\mathcal{X})$, the associated least squares estimator $\hat{f}_n$ has uniquely determined values $\hat{\theta}_{n1}, \ldots, \hat{\theta}_{nn}$ at the design points $X_1, \ldots, X_n$. For concreteness, it is extended to the whole of $\mathcal{X}$ by a suitable form of piecewise affine interpolation (Seijo and Sen, 2011). More precisely, in a pointwise sense, $\hat{f}_n$ is the largest convex function $h \colon \mathcal{X} \to \mathbb{R}$ satisfying $h(X_i) \leq \hat{\theta}_{ni}$ for $1 \leq i \leq n$, so that $\hat{f}_n$ is a polyhedral (i.e. finitely generated) convex function (Rockafellar, 1997, Corollary 19.1.2). We note for future reference that functions with a similar structure turn up in other multivariate convexity-constrained models, for example in log-concave maximum likelihood estimation.

Although a number of algorithms have been developed to compute univariate convex least squares estimators, it has proved more challenging to devise feasible procedures for multivariate convex regression. It was recognised by Seijo and Sen (2011) that in dimension d, the convex least squares problem can be formulated as a quadratic program with $n(n-1)$ constraints and $n(d+1)$ variables. The use of generic interior-point solvers was found to be impractical even for sample sizes n in the hundreds, so Mazumder et al. (2018) and latterly Chen and Mazumder (2020) have instead exploited problem-specific structure to obtain more efficient iterative procedures. In spite of the difficulties of dealing with $O(n^2)$ constraints, these algorithms were found to be able to handle instances where n and d are as large as 10^5 and 10 respectively.

Consistency results for multivariate convex least squares estimators were obtained by Seijo and Sen (2011) under mild regularity conditions in both fixed and random design settings. Until recently, very little was known about their finite-sample performance in dimensions $d \geq 2$. As we will see in Chapter 2, an important and interesting feature of multivariate shape-constrained estimators is that their performance often depends sensitively on the shape of the underlying domain. This usually necessitates a more careful and involved analysis than in univariate problems, and will undoubtedly be a focus of future research.

In a random design setting, Han and Wellner (2016a) obtained risk bounds for least squares estimators over subclasses $\mathcal{C}^B(\mathcal{X})$ of uniformly bounded convex functions defined on different convex bodies $\mathcal{X}$. They observed that the rates of convergence are faster when $\mathcal{X}$ is a polytope as opposed to a convex body with smooth boundary. Kur et al. (2019) showed that when $d \geq 4$ and $\mathcal{X}$ is the unit Euclidean ball, the bounded convex least squares estimator attains the minimax rate of order $n^{-2/(d+1)}$ over the classes $\mathcal{C}^B(\mathcal{X})$. By comparison, Kur et al. (2020) established that when $d \geq 5$ and $\mathcal{X}$ is a polytope with a constant number of facets, the bounded convex least squares estimator is rate suboptimal over $\mathcal{C}^B(\mathcal{X})$: its minimax risk over $\mathcal{C}^B(\mathcal{X})$ is essentially of the order $n^{-2/d}$, while the minimax rate for the estimation problem is of order $n^{-4/(d+4)}$.

Very recently, Kur et al. (2020) also derived the first known risk bounds for convex least squares estimators. For fixed lattice designs and polytopal domains $\mathcal{X}$, they proved that the convex least squares estimator over $\mathcal{C}(\mathcal{X})$ suffers the same rate suboptimality issue when $d \geq 5$, with a discrepancy between rates of order $n^{-2/d}$ and $n^{-4/(d+4)}$ as above. This is in stark contrast to the behaviour of the multivariate isotonic least squares estimator on $[0,1]^d$ discussed previously. It is still not known what happens to the convex least squares estimator when e.g. $\mathcal{X}$ is a Euclidean ball, or the isotonic least squares estimator when e.g. the (hyperrectangular) domain is not aligned with the coordinate axes.

1.2 Nonparametric maximum likelihood estimators for shape-constrained density estimation

Likelihood-based inference was pioneered by Fisher (1922) and is now a cornerstone of statistical theory and practice. In parametric models, results on the $(\sqrt{n})$-consistency, asymptotic normality and optimality of maximum likelihood estimators are well-known (e.g. van der Vaart, 1998). The same maximum likelihood paradigm can be applied to nonparametric density estimation problems, although care is needed to ensure that the resulting estimators are well-defined, and different tools are employed in their analysis.

In what follows, let $f_0 \colon \mathbb{R}^d \to [0,\infty)$ be an unknown d-dimensional density that we wish to estimate, and suppose that we observe $X_1,\dots,X_n \overset{\mathrm{iid}}{\sim} f_0$. Writing $\mathbb{P}_n := n^{-1}\sum_{i=1}^n \delta_{X_i}$ for the associated empirical distribution, recall that for any density $f \colon \mathbb{R}^d \to [0,\infty)$, the corresponding normalised log-likelihood is given by $\ell_n(f) := n^{-1}\sum_{i=1}^n \log f(X_i) = \int_{\mathbb{R}^d} \log f \, d\mathbb{P}_n$. For a class $\tilde{\mathcal{F}}$ of such densities, we then seek to define a *maximum likelihood estimator* $\hat{f}_n$ over $\tilde{\mathcal{F}}$ by

$$\hat{f}_n \in \operatorname*{argmax}_{f \in \tilde{\mathcal{F}}} \ell_n(f) = \operatorname*{argmax}_{f \in \tilde{\mathcal{F}}} \int_{\mathbb{R}^d} \log f \, d\mathbb{P}_n \tag{1.2.1}$$

when $\max_{f \in \tilde{\mathcal{F}}} \ell_n(f)$ exists and is finite. To solve the optimisation problem (1.2.1), it is sometimes helpful to relax the constraint that the functions in $\tilde{\mathcal{F}}$ integrate to 1. This can be done by introducing $\tilde{\mathcal{G}} := \{\lambda f : f \in \tilde{\mathcal{F}},\, \lambda > 0\}$ and a 'Lagrangian'

$$L(g, \mathbb{P}_n) := \int_{\mathbb{R}^d} \log g \, d\mathbb{P}_n - \int_{\mathbb{R}^d} g + 1 \tag{1.2.2}$$

for $g \in \tilde{\mathcal{G}}$. Even though there is no explicit Lagrange multiplier here, it can be seen that $\hat{f}_n$ maximises $g \mapsto L(g, \mathbb{P}_n)$ over $\tilde{\mathcal{G}}$ if and only if $\hat{f}_n$ maximises $f \mapsto \ell_n(f)$ over $\tilde{\mathcal{F}}$. Indeed, for all $\alpha \in \mathbb{R}$ and any $g \in \tilde{\mathcal{G}}$ with $L(g, \mathbb{P}_n) \in \mathbb{R}$, we have $e^\alpha g \in \tilde{\mathcal{G}}$ and $(\partial/\partial\alpha) L(e^\alpha g, \mathbb{P}_n) = 1 - e^\alpha \int_{\mathbb{R}^d} g$. Thus, $\alpha \mapsto L(e^\alpha g, \mathbb{P}_n)$ attains its unique maximum over $\mathbb{R}$ at $\alpha^* = \log(1/\int_{\mathbb{R}^d} g)$, whence $e^{\alpha^*} g \in \tilde{\mathcal{F}}$.

To ensure that there exists a maximiser $\hat{f}_n$ in (1.2.1), it is clear that suitable restrictions are needed on the class $\tilde{\mathcal{F}}$. Note that $\sup_{f \in \tilde{\mathcal{F}}} \ell_n(f) = \infty$ when $\tilde{\mathcal{F}}$ is the class of all (smooth) densities, or the class of all unimodal densities (with unknown mode) when $d = 1$; in these cases, $\tilde{\mathcal{F}}$ contains densities that can have arbitrarily tall spikes at one of the data points X_i whilst being uniformly bounded away from zero on $\{X_1, \dots, X_n\}$.

Nonparametric classes of densities $\tilde{\mathcal{F}}$ that admit maximum likelihood estimators include Sobolev classes (cf. Giné and Nickl, 2016, Chapter 7.2.3) and classes of Gaussian location mixtures (e.g. Kiefer and Wolfowitz, 1956; Saha and Guntuboyina, 2019), as well as the shape-constrained classes we will now discuss in more detail. There is some general machinery for establishing consistency, rates of convergence and limiting distributions for nonparametric maximum likelihood estimators; see for example van der Vaart and Wellner (1996), van de Geer (2000) and Patilea (2001).

1.2.1 Estimation of decreasing densities on the non-negative half line

A prototypical problem in shape-constrained inference is that of estimating a decreasing (i.e. non-increasing) density $f_0 \colon [0, \infty) \to [0, \infty)$. This arises naturally in many practical contexts, including pregnancy studies and mortality measurement. Motivated by the latter, Grenander (1956) proposed an estimator that bears his name and does not require the choice of any tuning parameters, in contrast to kernel and histogram estimators.

Characterisation and basic properties: Here, we take $\tilde{\mathcal{F}}$ in (1.2.1) to be the class $\mathcal{F}^{\downarrow}$ of all decreasing densities on $[0, \infty)$. It can be shown by elementary arguments that there is a unique maximum likelihood estimator $\hat{f}_n$ over $\mathcal{F}^{\downarrow}$, which is called the Grenander estimator, and moreover that $\hat{f}_n$ is a left continuous step function with jumps only at the observations X_i. In fact, $\hat{f}_n$ has an explicit representation; see for example Groeneboom and Jongbloed (2014, Lemma 2.2) or van der Vaart (1998, Lemma 24.5).

Proposition 1.2.1. *Let $\mathbb{F}_n \colon [0, \infty) \to [0, 1]$ be the empirical distribution function of $X_1, \dots, X_n$, so that $\mathbb{F}_n(x) := n^{-1} \sum_{i=1}^n \mathbb{1}_{\{X_i \le x\}}$ for $x \in [0, \infty)$. Then the Grenander estimator $\hat{f}_n$ is the left derivative of the least concave majorant $\hat{F}_n$ of $\mathbb{F}_n$.*

One interpretation of this (van der Vaart, 1998, Chapter 24) is that $\hat{f}_n$ is the result of applying a form of adaptive 'smoothing' to a rudimentary (and generally non-monotone) density estimator $\tilde{f}_n$ which takes the value $\{n(X_{(i)} - X_{(i-1)})\}^{-1}$ on $(X_{(i-1)}, X_{(i)}]$ for each $1 \le i \le n$, where $X_{(0)} := 0$ and $X_{(i)}$ is the i^{th} order statistic of $X_1, \dots, X_n$. Indeed, observe that $\hat{F}_n$ coincides with the least concave majorant of the function $\tilde{F}_n \colon [0, \infty) \to [0, 1]$ defined by $\tilde{F}_n(x) := \int_0^x \tilde{f}_n(s) \, ds$, so that $\hat{f}_n$ is obtained from $\tilde{f}_n$ by applying three operations, namely integrating, taking a least concave majorant and then differentiating (in that order).

On a related note, given the similarity between Proposition 1.2.1 and the characterisation of the univariate isotonic least squares estimator in Proposition 1.1.1, we can make the connection more concrete (cf. Yang and Barber, 2019, Section 5): set $Y_i := n(X_{(i)} - X_{(i-1)})$ for $1 \leq i \leq n$ and let $\hat{\theta}_n \equiv (\hat{\theta}_{n1}, \ldots, \hat{\theta}_{nn})$ be the isotonic least squares estimator over the monotone cone $\Theta^{\uparrow}$ in (1.1.9). Then for each $1 \leq i \leq n$, we have $\hat{f}_n(x) = 1/\hat{\theta}_{ni}$ for all $x \in (X_{(i-1)}, X_{(i)}]$, and $\hat{f}_n(x) = 0$ for all $x > X_{(n)}$.

Consistency: If the true density f_0 belongs to $\mathcal{F}^{\downarrow}$, then the corresponding distribution function F_0 is concave. A straightforward consequence of this is *Marshall's inequality* $\|\hat{F}_n - F_0\|_\infty \leq \|\mathbb{F}_n - F_0\|_\infty$ (Marshall, 1970), where we write $\|F\|_\infty := \sup_{x \in [0,\infty)} |F(x)|$ for $F \colon [0, \infty) \to \mathbb{R}$. Since $\|\mathbb{F}_n - F_0\|_\infty \to 0$ almost surely by the Glivenko–Cantelli theorem, it follows that $\|\hat{F}_n - F_0\|_\infty \to 0$ almost surely. Together with the concavity of F_0 and $\hat{F}_n$ for each n, this implies that $\hat{f}_n(x) \to f_0(x)$ almost surely as $n \to \infty$, for each $x \in (0, \infty)$ (Groeneboom and Jongbloed, 2014, Lemma 3.1). In addition, when f_0 is continuous on $(0, \infty)$, the pointwise consistency of $\hat{f}_n$ can be automatically upgraded to uniform consistency on closed subintervals of $(0, \infty)$ (Groeneboom and Jongbloed, 2014, Corollary 3.1). See Patilea (2001, Lemma 5.5) for an extension of these arguments to the misspecified case where $f_0 \notin \mathcal{F}^{\downarrow}$.

Asymptotic theory: Prakasa Rao (1969) proved that if $f_0 \in \mathcal{F}^{\downarrow}$ has a strictly negative derivative at some $x_0 \in (0, \infty)$, and $f_0(x_0) > 0$, then the Grenander estimator $\hat{f}_n$ of f_0 satisfies

$$n^{1/3}\bigl(\hat{f}_n(x_0) - f_0(x_0)\bigr) \xrightarrow{d} |4f_0(x_0)f_0'(x_0)|^{1/3}\,\mathcal{L}, \tag{1.2.3}$$

where $\mathcal{L}$ is the again the Chernoff distribution that appears in the limiting distribution (1.1.10) for the isotonic least squares estimator. For strictly decreasing, compactly supported and twice continuously differentiable $f_0 \in \mathcal{F}^{\downarrow}$, Groeneboom (1985) and Groeneboom et al. (1999) established an analogue of (1.2.3) for the L^1 distance between $\hat{f}_n$ and f_0, namely

$$n^{1/3} \int_0^\infty |\hat{f}_n(x) - f_0(x)|\,dx \xrightarrow{d} \biggl(\int_0^\infty |4f_0(x)f_0'(x)|^{1/3}\,dx\biggr)\,\mathbb{E}(U),$$

where $U \sim \mathcal{L}$. Further asymptotic results for L^p distances with $p \geq 1$ are also available (cf. Durot and Lopuhaä, 2018), and Hellinger convergence results under model misspecification can be found in Patilea (2001).

Boundary issues: As we saw above, the Grenander estimator $\hat{f}_n$ of $f_0 \in \mathcal{F}^{\downarrow}$ is strongly consistent at every $x \in (0, \infty)$. However, Woodroofe and Sun (1993) observed that $\hat{f}_n$ is inconsistent at 0, and instead proposed a penalised maximum likelihood approach to remedy this issue. The behaviour of $\hat{f}_n$ at the edge of the support of f_0 has been further elucidated by Kulikov and Lopuhaä (2006), who showed amongst other things that $\hat{f}_n(n^{-1/3})$ is $n^{1/3}$-consistent for estimating $f_0(0)$ if the right derivative of f_0 at 0 is strictly negative. Later, Balabdaoui et al. (2011) derived the limiting distributions of processes of the form $x \mapsto b_n\hat{f}_n(a_n x)$ for suitable sequences (a_n) and (b_n).

Estimation of convex, decreasing densities: A subclass of $\mathcal{F}^{\downarrow}$ that has also received some attention is the class $\mathcal{C}^{\downarrow}$ of all convex, decreasing densities on $[0, \infty)$. Groeneboom et al. (2001) verified that there is a unique maximum likelihood estimator $\hat{g}_n$ over $\mathcal{C}^{\downarrow}$, and moreover that $\hat{g}_n$ is a piecewise affine function with at most one knot in between any two successive observations (and no knots at the observations). Like the Grenander estimator, the maximum likelihood estimator $\hat{g}_n$ of some $g_0 \in \mathcal{C}^{\downarrow}$ is uniformly (strongly) consistent on closed subintervals of $(0, \infty)$ and inconsistent at 0. As for the pointwise asymptotics of $\hat{g}_n$, Groeneboom et al. (2001) showed that if $x_0 \in (0, \infty)$ is such that g_0'' exists and is continuous on a neighbourhood of x_0, with $g_0''(x_0) > 0$, then

$$\begin{pmatrix} n^{2/5}\bigl(\hat{g}_n(x_0) - g_0(x_0)\bigr) \\ n^{1/5}\bigl(\hat{g}_n'(x_0) - g_0'(x_0)\bigr) \end{pmatrix}$$

has a similar limiting distribution to the analogous quantity (1.1.12) in convex regression; here, this limit depends on $g_0(x_0)$ and $g_0''(x_0)$.

Least squares density estimators: We mention briefly that shape-constrained density estimators in the models above can also be obtained via a least squares approach, which minimises $f \mapsto Q_n(f) := \int_0^\infty f^2 - 2\int_{[0,\infty)} f\, d\mathbb{P}_n$ over the relevant class $\tilde{\mathcal{F}}$. The motivation for this is that if $\mathbb{P}_n$ actually had a Lebesgue density f_n, then minimising $f \mapsto Q_n(f)$ would amount to minimising $f \mapsto \int_0^\infty (f - f_n)^2$ over $\tilde{\mathcal{F}}$.

When $\tilde{\mathcal{F}} = \mathcal{F}^{\downarrow}$, it turns out that the least squares density estimator coincides with the Grenander estimator. On the other hand, if $\tilde{\mathcal{F}} = \mathcal{C}^{\downarrow}$, then the convex least squares estimator is different from the maximum likelihood estimator $\hat{g}_n$, although it has the same asymptotic behaviour (Groeneboom et al., 2001) and is easier to analyse. Moreover, the least squares estimator of some $g_0 \in \mathcal{C}^{\downarrow}$ satisfies a version of Marshall's inequality in which the right hand side is inflated by a factor of 2 (Dümbgen et al., 2007).

1.2.2 Log-concave density estimation

To prepare the ground for Chapter 2 of this thesis, we now discuss the constraint of log-concavity, which is applicable to multivariate as well as univariate densities. For $d \in \mathbb{N}$, a function $f\colon \mathbb{R}^d \to [0,\infty)$ is said to be log-concave if $\log f\colon \mathbb{R}^d \to [-\infty,\infty)$ is an (extended) concave function, where we set $\log 0 = -\infty$.

Properties of log-concave densities: The class $\mathcal{F}_d$ of all upper semi-continuous, log-concave densities on $\mathbb{R}^d$ lies at the heart of modern shape-constrained nonparametric inference, due to both the modelling flexibility it affords and its attractive stability properties (cf. Samworth, 2018; Saumard and Wellner, 2014; Walther, 2009). Indeed, $\mathcal{F}_d$ encompasses many standard parametric families, including Laplace, Gumbel, logistic, and certain beta, gamma and Weibull densities (Bagnoli and Bergstrom, 2005) when $d = 1$, as well as Gaussian densities and uniform densities on compact, convex sets for general $d \geq 1$. In addition, $\mathcal{F}_d$ is closed under marginalisation, convolution, conditioning and affine transformations (Prékopa, 1980), and can therefore be regarded as an infinite-dimensional surrogate for the class of d-dimensional Gaussian densities.

Log-concave densities have tails that decay at least exponentially fast, in the sense that for each $f \in \mathcal{F}_d$, there exist $a > 0$ and $b \in \mathbb{R}$ such that $f(x) \leq \exp(-a\|x\| + b)$ for all $x \in \mathbb{R}^d$ (Cule and Samworth, 2010, Lemma 1). In fact, for suitable choices of a and b that depend only on d, this bound holds uniformly over the class of *isotropic* log-concave densities with zero mean and identity covariance (e.g. Fresen, 2013, Lemma 13). We will show in Section 2.6.2 that when $d = 1$, we can in fact take $a = b = 1$ in the bound for the isotropic class, and that there is a natural sense in which these constants cannot be improved. Many other useful analytic properties of log-concave densities can be found in Lovász and Vempala (2006, Section 5).

Since a log-concave function is unimodal when restricted to any one-dimensional line, finite mixtures of log-concave densities are not necessarily log-concave: for example, when $p \in (0,1)$, the density of $pN_d(-\mu, I_d) + (1-p)N_d(\mu, I_d)$ belongs to $\mathcal{F}_d$ precisely when $\|\mu\| \leq 1$ (Cule et al., 2010). Thus, unlike the other shape-constrained function classes we have encountered so far, $\mathcal{F}_d$ is not convex.

The log-concave maximum likelihood estimator — structure and computation: To estimate a unknown $f_0 \in \mathcal{F}_d$ based on observations $X_1, \ldots, X_n \overset{\text{iid}}{\sim} f_0$, we can take $\tilde{\mathcal{F}} = \mathcal{F}_d$ in (1.2.1) and seek a maximum likelihood estimator $\hat{f}_n$ over $\mathcal{F}_d$. Cule et al. (2010, Theorem 2) established that if $n \geq d+1$, then $\hat{f}_n$ exists and is unique with probability 1, and that $\hat{f}_n$ is supported on the convex hull C_n of the data points $X_1, \ldots, X_n$ (which is a convex polytope). In fact, the proof also shows that there exist $y_1, \ldots, y_n \in \mathbb{R}$ such that in a pointwise sense, $\log \hat{f}_n$ is the minimal concave function $h \colon \mathbb{R}^d \to [-\infty, \infty)$ satisfying $h(X_i) \geq y_i$ for all $1 \leq i \leq n$. Thus, $\log \hat{f}_n$ is a special type of (piecewise affine) polyhedral concave function (Rockafellar, 1997, Corollary 19.1.2): it can be described as a 'tent function' whose graph is held up by 'tent poles' at the observations $X_1, \ldots, X_n$ with heights $y_1, \ldots, y_n$ respectively.

From a computational point of view, this observation is helpful because it can be used to reduce the original task of maximising (1.2.1) over the infinite-dimensional class $\mathcal{F}_d$ to a finite-dimensional convex optimisation problem over tent functions (Cule et al., 2010, Theorem 3), whose objective function σ is a slight alteration of (1.2.2). Although this is encouraging, a technical complication is that standard procedures such as Newton's method cannot be applied, in view of the fact that σ has points of non-differentiability. Roughly speaking, these occur at tent functions for which at least one of the corresponding tent poles is only just touching the roof of the tent, so that its removal leaves the tent structure unchanged. Nevertheless, an explicit subgradient of σ can still be computed at every point, based in part on a triangulation of the convex hull C_n into simplicial subdomains on which each tent function is affine (Cule et al., 2010, Proposition 5). Consequently, the log-concave maximum likelihood estimator $\hat{f}_n$ can be obtained by applying a variant of Shor's r-algorithm for convex, non-smooth optimisation, as implemented in the `R` package `LogConcDEAD` (Cule et al., 2009). This procedure is computationally feasible for sample sizes n in the order of 1000 when the dimension d is not too large. An alternative interior-point method has been proposed by Koenker and Mizera (2010).

When $d = 1$, there are faster algorithms for computing $\hat{f}_n$, including an active set algorithm called `logcondens` (Dümbgen and Rufibach, 2011) and a more recent constrained Newton method called `cnmlcd` (Liu and Wang, 2018). In this case, $\log \hat{f}_n$ is a piecewise affine function supported on the interval $[\min X_i, \max X_i]$, with knots only at the observations; compare this with the previously described structure of the maximum likelihood estimator of a convex, decreasing density.

Univariate asymptotic theory: By adapting and extending the techniques used in Groeneboom et al. (2001) to establish pointwise asymptotics in univariate convex function estimation, Balabdaoui, Rufibach and Wellner (2009) derived analogous results for the log-concave maximum likelihood estimator $\hat{f}_n$ of a log-concave density $f_0 \colon \mathbb{R} \to [0, \infty)$. Specifically, if $x_0 \in \mathbb{R}$ is such that $f_0(x_0) > 0$ and $\phi_0 := \log f_0$ is twice continuously differentiable on a neighbourhood of x_0, with $\phi_0''(x_0) < 0$, then

$$\begin{pmatrix} n^{2/5}\bigl(\hat{f}_n(x_0) - f_0(x_0)\bigr) \\ n^{1/5}\bigl(\hat{f}_n'(x_0) - f_0'(x_0)\bigr) \end{pmatrix}$$

has a non-degenerate limiting distribution that is constructed similarly to those in Groeneboom et al. (2001); here, this limit depends on $f_0(x_0)$ and $\phi_0''(x_0)$. As in the other univariate convexity-constrained models, $\hat{f}_n(x_0)$ and $\hat{f}_n'(x_0)$ achieve faster local rates of order $n^{-k/(2k+1)}$ and $n^{-(k-1)/(2k+1)}$ respectively at points x_0 where the 'local smoothness index' $k \in \mathbb{N}$ is larger than 2.

Under the conditions above, Deng et al. (2020) showed that there is a universal limiting distribution for the exact analogue of (1.1.13) for univariate log-concave density estimation. This facilitates the construction of asymptotically valid confidence intervals for $f_0(x_0)$ and $f_0'(x_0)$. As in other shape-constrained problems, little is known about pointwise limiting behaviour in multivariate log-concave density estimation, although a pointwise minimax lower bound of order $n^{-2/(d+4)}$ was established by Seregin and Wellner (2010) under a local smoothness condition of order 2.

Log-concave projections: To place log-concave maximum likelihood estimation within a broader framework, consider replacing the (random) empirical distribution $\mathbb{P}_n$ in (1.2.1) and (1.2.2) by a general probability distribution P on $\mathbb{R}^d$. Dümbgen et al. (2011, Theorem 2.2) showed that there exists a unique maximiser of $f \mapsto \int_{\mathbb{R}^d} \log f \, dP$ over $\mathcal{F}_d$ if and only if $P(H) < 1$ for any affine hyperplane $H \subseteq \mathbb{R}^d$ (i.e. 'the support of P is d-dimensional') and $\int_{\mathbb{R}^d} \|x\| \, dP(x) < \infty$. Writing $\mathcal{Q}_d$ for the set of all such distributions P, we can then define the *log-concave projection* $\psi^* \colon \mathcal{Q}_d \to \mathcal{F}_d$ by

$$\psi^*(P) := \operatorname*{argmax}_{f \in \mathcal{F}_d} \int_{\mathbb{R}^d} \log f \, dP.$$

Observe that if in addition $P \in \mathcal{Q}_d$ has a Lebesgue density f_P satisfying $\int_{\mathbb{R}^d} f_P \, |\log f_P| < \infty$, then $\psi^*(P)$ is the 'closest' element of $\mathcal{F}_d$ to f_P in the sense of minimising $f \mapsto \mathrm{KL}(f_P, f) := \int_{\mathbb{R}^d} f_P \log(f/f_P)$ over $\mathcal{F}_d$. In particular, if P has a density f_P that is log-concave, then $\psi^*(P) = f_P$. This is why we refer to ψ^* as a (Kullback–Leibler) projection onto $\mathcal{F}_d$, although since $\mathcal{F}_d$ is not convex and the Kullback–Leibler divergence is not a metric, ψ^* is different in nature to (and consequently harder to analyse than) ℓ_2 projections onto closed, convex sets. In particular, many techniques from the theory of shape-restricted regression (Section 1.1), such as those based on localised Gaussian widths (1.1.4) and statistical dimension (1.1.5), are not applicable in this setting.

An overall objective of this projection theory is to derive statistical properties of log-concave maximum likelihood estimators $\hat{f}_n = \psi^*(\mathbb{P}_n)$ (such as consistency and rates of convergence) by first establishing general analytic results about the deterministic map ψ^* (such as continuity) and then applying these directly to empirical distributions $\mathbb{P}_n$. This approach is based on convex analysis rather than the empirical process theory arguments used in standard consistency proofs, and as well as being mathematically clean, it yields guarantees for $\hat{f}_n$ under model misspecification (i.e. when the true density $f_0 \colon \mathbb{R}^d \to [0, \infty)$ is not log-concave). In Section 3.1 and 3.5.4, with the same aims in mind, we will develop an L^2 projection theory for a non-convex shape-constrained class of regression functions; the complication there is that due to a non-uniqueness issue, the projection map is set-valued.

Returning to the setting of log-concave density estimation, observe first that $\mathbb{P}_n$ belongs to $\mathcal{Q}_d$ if and only if the convex hull of $X_1, \dots, X_n \overset{\mathrm{iid}}{\sim} P_0$ is d-dimensional. When P_0 has a Lebesgue density, this occurs with probability 1 if and only if $n \geq d + 1$. Thus, we recover the earlier existence and uniqueness result for $\hat{f}_n$ (Cule et al., 2010, Theorem 2) as a special case of Dümbgen et al. (2011, Theorem 2.2). The map ψ^* has some other useful basic properties (Dümbgen et al., 2011, Remarks 2.3–2.6) that can be summarised as follows:

(i) ψ^* (and hence the estimator $\hat{f}_n$) is *affine equivariant*, in the sense that it commutes with affine transformations: pushing forward $P \in \mathcal{Q}_d$ by an affine transformation T and then applying ψ^* gives the same result as first applying ψ^* to P and then transforming according to T.

(ii) Let $P \in \mathcal{Q}_d$ and write P^* for the probability distribution with density $f^* := \psi^*(P)$. Then given any $\Delta \colon \mathbb{R}^d \to \mathbb{R}$ for which $e^{t\Delta} f^*$ is an integrable, log-concave function for sufficiently small $t > 0$, we have $\int_{\mathbb{R}^d} \Delta \, dP^* \geq \int_{\mathbb{R}^d} \Delta \, dP$. Indeed, by analogy with (1.2.2), f^* maximises $g \mapsto L(g, P) := \int_{\mathbb{R}^d} \log g \, dP - \int_{\mathbb{R}^d} g + 1$ over the class $\tilde{\mathcal{G}}_d := \{\lambda f : f \in \mathcal{F}_d, \lambda > 0\}$, so $0 \geq \lim_{t \searrow 0} t^{-1}\{L(e^{t\Delta} f^*, P) - L(f^*, P)\} = \int_{\mathbb{R}^d} \Delta \, dP - \int_{\mathbb{R}^d} \Delta \, dP^*$.

A consequence of this is that P^* is dominated by P in the convex ordering, in the sense that $\int_{\mathbb{R}^d} h \, dP^* \leq \int_{\mathbb{R}^d} h \, dP$ for all convex $h \colon \mathbb{R}^d \to (-\infty, \infty]$. In fact, using Strassen's theorem (Strassen, 1965), it can be shown that $A = 0$ if and only if P is log-concave (Samworth, 2018).

(iii) A consequence of (ii) is that P^* has the same mean as P but a smaller variance, in the sense that if $X \sim P$ and $X^* \sim P^*$, then $A := \mathrm{Cov}(X) - \mathrm{Cov}(X^*)$ is non-negative definite.

This motivates the definition of the *smoothed log-concave projection* $\tilde{\psi}^*(P)$ as the convolution of $\psi^*(P)$ and the Gaussian distribution $N_d(0, A)$ (Chen and Samworth, 2013; Dümbgen and Rufibach, 2009). It can be seen that $\tilde{\psi}^*(P)$ is an infinitely differentiable log-concave density that is supported on the whole of $\mathbb{R}^d$ and matches the first two moments of P.

(iv) The preimage of any $f \in \mathcal{F}_d$ under ψ^* is a convex subset of $\mathcal{Q}_d$.

In the special case where $d = 1$ and f is the standard Laplace density, this preimage contains all symmetric Pareto distributions with parameters α, σ satisfying $\sigma = \alpha - 1$, and is therefore an infinite-dimensional set (Samworth, 2018, Section 5.1).

In addition, Dümbgen et al. (2011) established continuity results for $\psi^*\colon \mathcal{Q}_d \to \mathcal{F}_d$ with respect to the L^1-Wasserstein metric W_1 on $\mathcal{Q}_d$; recall that for probability measures P, Q on $\mathbb{R}^d$, we define $W_1(P,Q) := \inf_{(X,Y)} \mathbb{E}(\|X - Y\|)$, where the infimum is taken over all pairs of random variables X, Y defined on a common probability space with $X \sim P$ and $Y \sim Q$. It is well-known that $W_1(P_n, P) \to 0$ if and only if $P_n \xrightarrow{d} P$ and $\int_{\mathbb{R}^d} \|x\|\, dP_n(x) \to \int_{\mathbb{R}^d} \|x\|\, dP(x)$.

Theorem 1.2.2 (Dümbgen et al., 2011, Theorem 2.15 and Remark 2.16)**.** *For $P \in \mathcal{Q}_d$, define $f^* := \psi^*(P)$ and its support* $\mathrm{supp}(f^*) := \{x \in \mathbb{R}^d : f^*(x) > 0\}$*. Let (P_n) be a sequence of probability measures on $\mathbb{R}^d$ satisfying $W_1(P_n, P) \to 0$. Then $P_n \in \mathcal{Q}_d$ and $f_n^* := \psi^*(P_n)$ is well defined for all sufficiently large n, and the following hold:*

(i) Pointwise and uniform convergence*: $f_n^*(x) \to f^*(x)$ for all $x \in \mathbb{R}^d$ that do not lie on the boundary of* $\mathrm{supp}(f^*)$*, and in fact $f_n^* \to f^*$ uniformly on all closed sets consisting of continuity points of f^*.*

(ii) Convergence in exponentially weighted total variation norms*: if $a > 0$ and $b \in \mathbb{R}$ are such that $f^*(x) \le \exp(-a\|x\| + b)$ for all $x \in \mathbb{R}^d$, as in Cule and Samworth (2010, Lemma 1), then $\int_{\mathbb{R}^d} e^{a'\|x\|} |f_n^* - f^*| \to 0$ for any $a' < a$.*

Remark 1.2.1. By taking $a' = 0$ in (ii), we see that $f_n^* \to f^*$ in total variation. Equivalently, $d_{\mathrm{H}}(f_n^*, f^*) \to 0$, where

$$d_{\mathrm{H}}(f,g) := \biggl\{\int_{\mathbb{R}^d} (\sqrt{f} - \sqrt{g})^2\biggr\}^{1/2} \tag{1.2.4}$$

is the *Hellinger distance* between densities f and g.

As mentioned previously, Theorem 1.2.2 is a deterministic result that can in particular be applied to a sequence of empirical distributions $(\mathbb{P}_n)$ corresponding to (the first n terms of) a sequence of i.i.d. observations $X_1, X_2, \ldots$ from some $P_0 \in \mathcal{Q}_d$, which need not have a log-concave density. Indeed, $W_1(\mathbb{P}_n, P_0) \to 0$ almost surely since $\int_{\mathbb{R}^d} \|x\|\, d\mathbb{P}_n \to \int_{\mathbb{R}^d} \|x\|\, dP_0$ almost surely by the strong law of large numbers and $\mathbb{P}_n \xrightarrow{d} P_0$ almost surely by Varadarajan's theorem (Dudley, 2002, Theorem 11.4.1); alternatively, this Wasserstein convergence follows from bracketing entropy bounds which imply that the class of all Lipschitz $h\colon \mathbb{R}^d \to \mathbb{R}$ (with $h(0) = 0$) is P_0-Glivenko–Cantelli when $P_0 \in \mathcal{Q}_d$ (van der Vaart, 1994, Corollary 4.1). It therefore follows immediately that the convergence statements in Theorem 1.2.2 hold almost surely for the corresponding sequence of log-concave maximum likelihood estimators $\hat{f}_n = \psi^*(\mathbb{P}_n)$. In summary, $(\hat{f}_n)$ is strongly consistent when P_0 has a log-concave density f_0 and $\psi^*(P_0) = f_0$, and robust to misspecification in general when the limiting $\psi^*(P_0)$ is not a density for P_0 but rather the 'closest' element of $\mathcal{F}_d$ to P_0 in a Kullback–Leibler sense.

It turns out that the map ψ^* is not continuous with respect to the coarser topology of weak convergence on $\mathcal{Q}_d$ (Dümbgen et al., 2011, Remark 2.17), and moreover that ψ^* is not uniformly continuous with respect to W_1 (Samworth, 2018, page 501). While Theorem 1.2.2 is stated and proved as a asymptotic result, Barber and Samworth (2021) recently established a more quantitative version of Remark 1.2.1 which shows that $\psi^*\colon (\mathcal{Q}_d, W_1) \to (\mathcal{F}_d, d_{\mathrm{H}})$ is locally (1/4)-Hölder continuous. More precisely, for $P \in \mathcal{Q}_d$, they define $\epsilon_P := \inf_{u \in \mathbb{S}^{d-1}} \mathbb{E}\bigl(|u^\top (X - \mu_P)|\bigr)$, where $X \sim P$ and $\mu_P := \mathbb{E}(X)$, and show that $\epsilon_P > 0$. Their main result is that there exists $C_d > 0$ depending only on d such that

$$d_{\mathrm{H}}\bigl(\psi^*(P), \psi^*(Q)\bigr) \le C_d \left(\frac{W_1(P,Q)}{\epsilon_P \vee \epsilon_Q}\right)^{1/4} \tag{1.2.5}$$

for all $P, Q \in \mathcal{Q}_d$; a matching lower bound shows that the dependence of this bound on $W_1(P,Q)$ and ϵ_P, ϵ_Q cannot be improved. When $X_1, \ldots, X_n \overset{\mathrm{iid}}{\sim} P_0$ for a distribution P_0 on $\mathbb{R}^d$ with a finite q^{th} moment for some $q > 1$ but not necessarily a log-concave density, applying (1.2.5) to the empirical distribution $\mathbb{P}_n$ yields a finite-sample squared Hellinger risk bound of order $n^{-\min\left(\frac{1}{2d}, \frac{1}{2} - \frac{1}{2q}\right)} \log^{3/2} n$ for the log-concave maximum likelihood estimator $\hat{f}_n = \psi^*(\mathbb{P}_n)$. Thus, the rate of convergence of $\hat{f}_n$ to $\psi^*(P_0)$ can be quantified even under misspecification. Complementary lower bounds show that these rates can be much slower than in the correctly specified settings we go on to discuss. For example, in the case $d = 1$ (where the risk bound above is actually obtained by a different argument), the minimax rate over $\mathcal{F}_d$ with respect to d_{H}^2 is of order $n^{-4/5}$, but rates under misspecification can be slower than $n^{-1/2}$.

Risk bounds: Kim and Samworth (2016) proved the following minimax lower bound for the problem of estimating an unknown log-concave density $f_0 \in \mathcal{F}_d$ based on $X_1, \ldots, X_n \overset{\mathrm{iid}}{\sim} f_0$: for each $d \in \mathbb{N}$, there exists $c_d > 0$[†] such that

$$\inf_{\tilde{f}_n} \sup_{f_0 \in \mathcal{F}_d} \mathbb{E}\{d_{\mathrm{H}}^2(\tilde{f}_n, f_0)\} \ge \begin{cases} c_1\, n^{-4/5} & \text{if } d = 1 \\ c_d\, n^{-2/(d+1)} & \text{if } d \ge 2, \end{cases} \tag{1.2.6}$$

where the infimum is taken over all estimators $\tilde{f}_n$ of f_0 based on $X_1, \ldots, X_n$. Thus, when $d \ge 3$, there is a more severe curse of dimensionality than for the problem of estimating a density with two bounded derivatives and exponentially decaying tails, for which the corresponding minimax rate is $n^{-4/(d+4)}$ in all dimensions (Goldenshluger and Lepski, 2014). See Section 2.8.2 for further details and discussion. The reason why this comparison is interesting is because any concave function is twice differentiable Lebesgue almost everywhere on its effective domain, while a twice differentiable function is concave if and only if its Hessian matrix is non-positive definite at every point. This observation had led to the prediction that the rates in these problems ought to coincide (e.g. Seregin and Wellner, 2010, page 3778).

The result (1.2.6) is relatively discouraging as far as high-dimensional log-concave density estimation is concerned, and has motivated the definition of alternative procedures that seek improved rates when d is large under additional structure, such as independent component analysis (Samworth and Yuan, 2012) or symmetry[‡] (Xu and Samworth, 2021). Nevertheless, in lower-dimensional settings, the performance of the log-concave maximum likelihood estimator $\hat{f}_n$ has been studied with respect to the divergence

$$d_X^2(\hat{f}_n, f_0) := n^{-1} \sum_{i=1}^n \log \frac{\hat{f}_n(X_i)}{f_0(X_i)} \tag{1.2.7}$$

[†]In fact, more recently, Kur et al. (2019) proved that c_d may be chosen independently of the dimension d.

[‡]Xu and Samworth (2021) consider the subclass of all K-*homothetic* densities in $f \in \mathcal{F}_d$ for some known or unknown convex body $K \subseteq \mathbb{R}^d$; these satisfy $f(x) = g(\rho_K(x))$ for some $g\colon [0,\infty) \to [0,\infty)$, where ρ_K is the Minkowski functional of K (defined in Section 1.4). When K is a Euclidean ball or an ellipsoid, the K-homothetic densities are precisely those that are spherically or elliptically symmetric respectively.

defined on page 2281 of Kim et al. (2018). This loss function is an empirical analogue of the Kullback–Leibler divergence $\mathrm{KL}(\hat{f}_n, f_0)$, where

$$\mathrm{KL}(f,g) := \int_{\mathbb{R}^d} f \log\left(\frac{f}{g}\right), \tag{1.2.8}$$

and in fact

$$d_{\mathrm{H}}^2(\hat{f}_n, f_0) \leq \mathrm{KL}(\hat{f}_n, f_0) \leq d_{\mathrm{X}}^2(\hat{f}_n, f_0).$$

Here, the first bound is standard, while the second inequality is specific to $\hat{f}_n$ and follows by applying property (ii) on page 14 (Dümbgen et al., 2011, Remark 2.3) to the function $\Delta\colon x \mapsto \log\bigl(f_0(x)/\hat{f}_n(x)\bigr)$; indeed, for $t \in [0,1]$, the function $e^{t\Delta}\hat{f}_n = \exp\bigl((1-t)\log \hat{f}_n + t \log f_0\bigr) \leq (1-t)\hat{f}_n + tf_0$ is integrable (by the convexity of $z \mapsto e^z$), and $(1-t)\log \hat{f}_n + t\log f_0$ is concave. A small modification of the proof of Kim and Samworth (2016, Theorem 5) yields the following result, which is stated as Theorem 2.6.2 in Section 2.6.1 for convenience:

$$\sup_{f_0 \in \mathcal{F}_d} \mathbb{E}\{d_{\mathrm{X}}^2(\hat{f}_n, f_0)\} = \begin{cases} O(n^{-4/5}) & \text{if } d = 1 \\ O(n^{-2/3}\log n) & \text{if } d = 2 \\ O(n^{-1/2}\log n) & \text{if } d = 3; \end{cases} \tag{1.2.9}$$

see also Doss and Wellner (2016) for a related result in the univariate case. When $d = 2$, the $\log n$ term can in fact be improved to $\log^{2/3} n$ (Han, 2021). Moreover, very recently, Kur et al. (2019) proved that[§]

$$\sup_{f_0 \in \mathcal{F}_d} \mathbb{E}\{d_{\mathrm{H}}^2(\hat{f}_n, f_0)\} = O_d(n^{-2/(d+1)}\log n) \tag{1.2.10}$$

for $d \geq 4$, so that, at least in squared Hellinger loss, it follows from (1.2.6), (1.2.9) and (1.2.10) that $\hat{f}_n$ attains the minimax optimal rate in all dimensions, up to a logarithmic factor.

The worst-case rates of convergence in (1.2.9) and (1.2.10) have now been extended to classes of *s-concave densities* on $\mathbb{R}^d$ (e.g. Doss and Wellner, 2016; Han and Wellner, 2016b; Koenker and Mizera, 2010; Seregin and Wellner, 2010). When $s < 0$, these encompass heavier-tailed distributions that are excluded from the log-concave class (which corresponds to $s = 0$); for example, when $d = 1$, t-distributions with ν degrees of freedom are s-concave for $s \leq -1/(\nu+1)$. Han (2021, Theorem 3.7) proved that if $d \geq 2$ and $g_0\colon \mathbb{R}^d \to [0,\infty)$ is an s-concave density with $s > -1/d$, then the s-concave maximum likelihood estimator $\hat{g}_n$ satisfies

$$d_{\mathrm{H}}^2(\hat{g}_n, g_0) = O_p\bigl(n^{-2/(d+1)}\log^{\alpha_d} n\bigr),$$

where $\alpha_2 := 2/3$, $\alpha_3 := 2$ and $\alpha_d := 1$ for $d \geq 4$.

1.3 Adaptation of shape-constrained estimators

One of the most intriguing aspects of many shape-constrained estimators is their ability to *adapt* to unknown features of the underlying data generating mechanism. To illustrate what we mean by this, consider a general setting in which the goal is to estimate a function or parameter that belongs to a class $\mathcal{D}$. Given a subclass $\mathcal{D}' \subseteq \mathcal{D}$, we say that our estimator adapts to $\mathcal{D}'$ with respect to a given loss function if its worst-case rate of convergence over $\mathcal{D}'$ is an improvement on its corresponding worst-case rate over $\mathcal{D}$; in the best case, it may even attain the minimax rates of convergence over both $\mathcal{D}'$ and $\mathcal{D}$, at least up to polylogarithmic factors in the sample size.

[§]Here and below, the $O_d(\cdot)$ notation is used as shorthand for an upper bound that holds up to a dimension-dependent quantity.

Univariate results: As a result of intensive work over the past decade, the adaptive behaviour of shape-constrained estimators is now fairly well understood in a variety of univariate problems (Balabdaoui, Rufibach and Wellner, 2009; Chatterjee et al., 2015; Chatterjee and Lafferty, 2019; Dümbgen and Rufibach, 2009; Jankowski, 2014; Kim et al., 2018). To give a concrete example, we consider once again the univariate isotonic least squares estimator $\hat{\theta}_n$ over the monotone cone $\mathcal{D} \equiv \Theta^{\uparrow}$ in (1.1.9), and recall from (1.1.11) that $\hat{\theta}_n$ attains the minimax rate of $O(n^{-2/3})$ for signals $\theta_0 \in \Theta^{\uparrow}$ of bounded uniform norm. On the other hand, the fact that the least squares estimator is piecewise constant motivates the thought that $\hat{\theta}_n$ might adapt to piecewise constant signals. More precisely, taking $\mathcal{D}' \equiv \Theta^{\uparrow}_k$ to be the subclass consisting of signals in $\Theta^{\uparrow}$ with at most k constant pieces, Bellec (2018, Theorem 3.2) established the risk bound

$$R(\hat{\theta}_n, \theta_0) \leq \inf_{\theta \in \Theta^{\uparrow}_k} \left\{ \frac{1}{n} \|\theta - \theta_0\|^2 + \frac{k}{n} \log\left(\frac{en}{k}\right) \right\} \tag{1.3.1}$$

when the noise variables $\xi_1, \ldots, \xi_n$ (1.1.2) are independent sub-Gaussian random variables with parameter 1. This holds for all $\theta_0 \in \mathbb{R}^n$, so model misspecification is allowed, and if θ_0 is (well-approximated by) an element of $\Theta^{\uparrow}_k$, then we (essentially) obtain a bound of $(k/n)\log(en/k)$. Up to the logarithmic factor, this rate of convergence (which is parametric when k is a constant) is the same as could be attained by an 'oracle' estimator that had access to the locations of the jumps in the signal. This beautiful sharp oracle inequality (1.3.1) relies crucially on the characterisation of the least squares estimator as an ℓ_2 projection onto the closed, convex cone $\Theta^{\uparrow}$; indeed, it is obtained as a special case of the general result (1.1.7) by substituting in the exact formula $\delta(\Theta^{\uparrow}) = \sum_{j=1}^{n} 1/j$ in (1.1.8) for the statistical dimension (1.1.5) of the monotone cone.

Multivariate results: In the special cases of isotonic and convex regression, recent work has shown that shape-constrained least squares estimators exhibit an even richer range of adaptation properties in higher dimensions (Chatterjee et al., 2018; Deng and Zhang, 2020; Han, 2021; Han et al., 2019; Han and Wellner, 2016a; Pananjady and Samworth, 2020). For instance, Chatterjee et al. (2018) showed that the least squares estimator in bivariate isotonic regression continues to enjoy parametric adaptation up to polylogarithmic factors when the signal is constant on a small number of rectangular pieces. On the other hand, Han et al. (2019) proved that, in general dimensions $d \geq 3$, the least squares estimator in fixed, lattice design isotonic regression¶ adapts at rate $\tilde{O}(n^{-2/d})$ for constant signals, and that it is not possible to obtain a faster rate for this estimator. This is still an improvement on the minimax rate of $\tilde{O}(n^{-1/d})$ over all isotonic signals (in the lexicographic ordering) with bounded uniform norm, but is strictly slower than the parametric rate. We remark that, in addition to the ideas employed by Bellec (2018), these higher-dimensional results rely on an alternative characterisation of the least squares estimator due to Chatterjee (2014), as well as an argument that controls the statistical dimension of the d-dimensional monotone cone by induction on d; see Han (2021, Theorem 3.9) for an alternative approach to the latter in random designs. Given the surprising nature of these results, it is of great interest to understand the extent to which adaptation is possible in other shape-constrained estimation problems.

1.4 Notation and convex analysis background

Throughout the rest of the thesis, our theoretical treatment of convexity-constrained estimators relies heavily on tools from convex analysis, so in this subsection, we review the relevant concepts. Accessible introductions to much of this material can be found in Schneider (2014) and Rockafellar (1997).

¶Here and below, the $\tilde{O}$ notation is used to denote rates that hold up to polylogarithmic factors in n.

For a fixed $d \in \mathbb{N}$, we write $\{e_1, \ldots, e_d\}$ for the standard basis of $\mathbb{R}^d$ and denote the ℓ_2 norm of $x = (x_1, \ldots, x_d) = \sum_{j=1}^d x_j e_j \in \mathbb{R}^d$ by $\|x\| \equiv \|x\|_2 = \bigl(\sum_{j=1}^d x_j^2\bigr)^{1/2}$. For $x, y \in \mathbb{R}^d$, let $[x, y] := \{tx + (1-t)y : t \in [0,1]\}$ denote the closed line segment between them, and define (x, y), $[x, y)$, $(x, y]$ analogously. For $x \in \mathbb{R}^d$ and $r > 0$, let $\bar{B}(x, r) := \{w \in \mathbb{R}^d : \|w - x\| \leq r\}$ and $B(x, r) := \{w \in \mathbb{R}^d : \|w - x\| < r\}$. Recall that a *line* is a set of the form $\{x + \lambda u : \lambda \in \mathbb{R}\}$ and that a *ray* is a set of the form $\{x + \lambda u : \lambda \geq 0\}$, where $x \in \mathbb{R}^d$ and $u \in \mathbb{R}^d \setminus \{0\}$.

For $A \subseteq \mathbb{R}^d$, let $\operatorname{conv} A$, $\operatorname{aff} A$, $\operatorname{span} A$ respectively denote the convex hull, affine hull and linear span of A. We write $\dim(A)$ for the *affine dimension* of A, i.e. the dimension of the affine hull of A, and for Lebesgue-measurable $A \subseteq \mathbb{R}^d$, we write $\mu_d(A)$ for the d-dimensional Lebesgue measure of A. If $0 < \dim(A) = k < d$, we can view A as a subset of its affine hull and define $\mu_k(A)$ analogously, whilst also setting $\mu_l(A) = 0$ for each integer $l > k$. In addition, we denote the set of positive definite $d \times d$ matrices by $\mathbb{S}^{d \times d}$ and the $d \times d$ identity matrix by $I \equiv I_d$.

A *cone* is a set $C \subseteq \mathbb{R}^d$ with the property that $\lambda C \subseteq C$ for all $\lambda > 0$. We say that C is *pointed* if $C \cap (-C) = \{0\}$. If C is a non-empty, closed, convex cone, then the *dual cone* $C^* := \{\alpha \in \mathbb{R}^d : \alpha^\top x \geq 0 \text{ for all } x \in C\}$ is also closed and convex, and we have $C^{**} = C$ (Schneider, 2014, Theorem 1.6.1).

If $E \subseteq \mathbb{R}^d$ is non-empty and convex, then its *relative interior* $\operatorname{relint} E$ is defined as the interior of E within the ambient space $\operatorname{aff} E$, and we write $\partial E := (\operatorname{Cl} E) \setminus (\operatorname{relint} E)$ for the *relative boundary* of E. It is always the case that $\partial E = \partial(\operatorname{Cl} E)$ and $\mu_d(\partial E) = 0$; see Schneider (2014, Theorem 1.1.15(c)) and Lang (1986) for example. If in addition E is closed, then the *recession cone* $\operatorname{rec}(E) := \{u \in \mathbb{R}^d : E + u \subseteq E\}$ is closed and convex, and we have $\operatorname{rec}(E) = \{0\}$ if and only if E is compact (Rockafellar, 1997, Theorem 8.4).

A *closed half-space* is a set of the form $\{x \in \mathbb{R}^d : \alpha^\top x \leq u\}$, where $\alpha \in \mathbb{R}^d \setminus \{0\}$ and $u \in \mathbb{R}$, and the interiors and boundaries of closed half-spaces are known as *open half-spaces* and *affine hyperplanes* respectively. For a non-empty and convex $E \subseteq \mathbb{R}^d$, we say that an affine hyperplane H *supports* E if $H \cap E \neq \emptyset$ and H is the boundary of a closed half-space that contains E. A *face* $F \subseteq E$ is a convex set with the property that if $u, v \in E$ and $tu + (1-t)v \in F$ for some $t \in (0,1)$, then $u, v \in F$. We say that $x \in E$ is an *extreme point* if $\{x\}$ is a face of E. Also, we say that $F \subseteq E$ is an *exposed face* of E if $F = E \cap H$ for some affine hyperplane H that supports E. Exposed faces of affine dimensions 0, 1 and $\dim(E) - 1$ are also known as *exposed points* (or *vertices*), *edges* and *facets* respectively. We write $\mathcal{F}(E)$ for the set of all facets of E.

Let $\mathcal{K} \equiv \mathcal{K}_d$ denote the collection of all closed, convex sets $K \subseteq \mathbb{R}^d$ with non-empty interior, and let $\mathcal{K}^b \equiv \mathcal{K}_d^b$ be the collection of all bounded $K \in \mathcal{K}_d$. We say that $K \in \mathcal{K}$ is *line-free* if K does not contain a line; i.e. for all $x \in K$ and $u \in \mathbb{R}^d \setminus \{0\}$, there exists some $\lambda \in \mathbb{R}$ such that $x + \lambda u \notin K$. Also, if $K \in \mathcal{K}$, then $K = \operatorname{Cl} \operatorname{Int} K$ (Schneider, 2014, Theorem 1.1.15(b)) and $\operatorname{Exp} K \subseteq \operatorname{Ext} K$, where $\operatorname{Ext} K$ and $\operatorname{Exp} K$ respectively denote the sets of extreme points and exposed points of K. For $K \in \mathcal{K}$, Straszewicz's theorem (Schneider, 2014, Theorem 1.4.7) asserts that $\operatorname{Ext} K \subseteq \operatorname{Cl} \operatorname{Exp} K$. Moreover, for each $K \in \mathcal{K}$ with $0 \in \operatorname{Int} K$, the *Minkowski functional* of K is the function $\rho_K \colon \mathbb{R}^d \to [0, \infty)$ defined by $\rho_K(x) := \inf\{\lambda > 0 : x \in \lambda K\}$, which is easily seen to be positively homogeneous (i.e. $\rho_K(\lambda x) = \lambda \rho_K(x)$ for all $\lambda > 0$ and $x \in \mathbb{R}^d$) and subadditive (i.e. $\rho_K(x + y) \leq \rho_K(x) + \rho_K(y)$ for all $x, y \in \mathbb{R}^d$), and therefore convex; see Schneider (2014, Section 1.7) for example.

A *polyhedral set* is a subset of $\mathbb{R}^d$ that can be expressed as the intersection of finitely many closed half-spaces, and a *polytope* is a bounded polyhedral set, or equivalently the convex hull of a finite subset of $\mathbb{R}^d$; see Theorems 2.4.3 and 2.4.6 in Schneider (2014). As a special case, we also view $\mathbb{R}^d$ as a polyhedral set with 0 facets. Let $\mathcal{P} \equiv \mathcal{P}_d$ denote the collection of all polyhedral sets in $\mathbb{R}^d$ with non-empty interior, and for $m \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, let $\mathcal{P}^m \equiv \mathcal{P}_d^m$ denote the collection of all $P \in \mathcal{P}$ with at most m facets. For $1 \leq k \leq d$, a *k-parallelotope* is the image of $[0,1]^k$ under an injective affine transformation from $\mathbb{R}^k$ to $\mathbb{R}^d$, i.e. a polytope of the form $\{v_0 + \sum_{\ell=1}^k \lambda_\ell v_\ell : 0 \leq \lambda_\ell \leq 1 \text{ for all } \ell\}$, where $v_0, v_1, \ldots, v_k \in \mathbb{R}^d$ and $v_1, \ldots, v_k$ are linearly independent. Recall also that a *k-simplex* is the convex hull of $k+1$ affinely independent points in $\mathbb{R}^d$. Finally, for $P \in \mathcal{P}_d$, a *(polyhedral) subdivision* of P is a finite collection of sets $E_1, \ldots, E_\ell \in \mathcal{P}_d$ such that $P = \bigcup_{j=1}^{\ell} E_j$ and $E_i \cap E_j$ is a common face of E_i and E_j for all $i, j \in \{1, \ldots, \ell\}$. A *triangulation* of a polytope $P \in \mathcal{P}_d$ is a subdivision of P consisting solely of d-simplices.

Finally, if $f \colon S \to \mathbb{R} \cup \{\infty\}$ is a function whose domain S is a subset of $\mathbb{R}^d$, then the *epigraph* of f is the set $\{(x,t) \in S \times \mathbb{R} : f(x) \leq t\}$.

Comment on notation: For the avoidance of confusion, we mention here that while concepts and definitions from this chapter are used throughout the thesis, any additional notation should be considered to be specific to the chapter in which it is introduced. For example, $\mathcal{F}^1$ appears in both Chapters 2 and 3 but refers to two entirely different function classes.

Chapter 2

Adaptation in multivariate log-concave density estimation

2.1 Introduction

This chapter concerns multivariate adaptation behaviour in log-concave density estimation. Let $\mathcal{F}_d$ denote the class of upper semi-continuous, log-concave densities on $\mathbb{R}^d$. For independent and identically distributed random vectors $X_1, \ldots, X_n$ with density $f_0 \in \mathcal{F}_d$, we write $\hat{f}_n := \mathrm{argmax}_{f \in \mathcal{F}_d} \sum_{i=1}^n \log f(X_i)$ for the corresponding log-concave maximum likelihood estimator; see Section 1.2.2. Recall from (1.2.7) that we write $d_X^2(\hat{f}_n, f_0) = n^{-1} \sum_{i=1}^n \log \frac{\hat{f}_n(X_i)}{f_0(X_i)}$. Our goal is to explore the potential of $\hat{f}_n$ to adapt to three different types of subclass of $\mathcal{F}_d$, in the sense of Section 1.3. The definition of the first of these is motivated by the observation that $\log \hat{f}_n$ is piecewise affine on the convex hull of $X_1, \ldots, X_n$, a polyhedral subset of $\mathbb{R}^d$ (Cule et al., 2010). It is therefore natural to consider, for $k \in \mathbb{N}$ and $m \in \mathbb{N} \cup \{0\}$, the subclass $\mathcal{F}^k(\mathcal{P}^m) \equiv \mathcal{F}_d^k(\mathcal{P}^m) \subseteq \mathcal{F}_d$ consisting of densities that are both log-k-affine on their support (see Section 2.1.1), and have the property that this support is a polyhedral set with at most m facets. Note that this class contains densities with unbounded support. By Proposition 2.2.1 in Section 2.2 below, the complexity of such densities f can be measured in terms of the sum $\Gamma(f)$ of the numbers of facets of the subdomains in the polyhedral subdivision of the support induced by f. A consequence of our first main result, Theorem 2.2.2, is that for all $f_0 \in \mathcal{F}^k(\mathcal{P}^m)$, we have

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} = \tilde{O}\left(\frac{\Gamma(f_0)}{n}\right) \tag{2.1.1}$$

when $d \in \{2, 3\}$; moreover, we also show that $\Gamma(f_0)$ is at most of order $k + m$ when $d = 2$, and at most of order $k(k+m)$ when $d = 3$. Thus, when k and m may be regarded as constants, (2.1.1) reveals that, up to the polylogarithmic term, the log-concave maximum likelihood estimator adapts at a parametric rate to $\mathcal{F}^k(\mathcal{P}^m)$ when $d \in \{2, 3\}$. Moreover, Theorem 2.2.2 offers a complete picture for this type of adaptation by providing a sharp oracle inequality that covers the case where f_0 is well approximated (in a Kullback–Leibler sense) by a density in $\mathcal{F}^k(\mathcal{P}^m)$ for some k, m. Unsurprisingly, the proof of this inequality is much more delicate and demanding than the corresponding univariate result given in Kim et al. (2018), owing to the greatly increased geometric complexity of both the boundaries of convex subsets of $\mathbb{R}^d$ for $d \geq 2$ and the structure of the polyhedral subdivisions induced by the densities in $\mathcal{F}^k(\mathcal{P}^m)$. In particular, the parameter m plays no role in the univariate problem, since the boundary of a convex subset of the real line has at most two points, but it turns out to be crucial in this multivariate setting. Indeed, no form of adaptation would be achievable in the absence of restrictions on the shape of the support of $f_0 \in \mathcal{F}_d$; for instance, when f_0 is the uniform density on a closed Euclidean ball in $\mathbb{R}^d$ with $d \geq 2$, consideration of the volume of the convex hull of $X_1, \ldots, X_n$ yields that $\mathbb{E}\{d_{\mathrm{H}}^2(\hat{f}_n, f_0)\} \geq \tilde{c}_d\, n^{-2/(d+1)}$ for some $\tilde{c}_d > 0$ depending only on d (Wieacker, 1987).

In contrast to the isotonic regression problem described in Section 1.3, Theorem 2.2.2 indicates that even when $d = 3$, the log-concave maximum likelihood estimator also enjoys essentially parametric adaptation when f_0 is close to a density in $\mathcal{F}^k(\mathcal{P}^m)$ for small k and m. Unfortunately, our arguments do not allow us to extend our results to dimensions $d \geq 4$, where the relevant bracketing entropy integral diverges at a polynomial rate. Recent work by Carpenter et al. (2018) derived worst-case rates in squared Hellinger loss for the log-concave maximum likelihood estimator when $d \geq 4$; the crux of their argument involved using Vapnik–Chervonenkis theory to bound

$$\mathbb{E}\biggl(\sup_{K \in \mathcal{K}_d^*} \biggl| \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{X_i \in K\}} - \mathbb{P}(X_1 \in K) \biggr| \biggr),$$

where $\mathcal{K}_d^*$ denotes the set of all closed, convex subsets of $\mathbb{R}^d$. Kur et al. (2019) obtained an improved bound on this quantity of $O_d(n^{-2/(d+1)})$ using a general chaining argument, and this allowed them to deduce the worst-case guarantees on the performance of the log-concave maximum likelihood estimator stated in (1.2.10). Unfortunately, it is unclear whether this approach can provide any adaptation guarantees.

Sections 2.3 and 2.4 consider different subclasses of $\mathcal{F}_d$, and are motivated by the hope that if we rule out 'bad' log-concave densities such as the uniform densities with smooth boundaries mentioned above, then we may be able to achieve faster rates of convergence, up to the $n^{-4/(d+4)}$ rate conjectured by Seregin and Wellner (2010). Since this rate already coincides with the worst-case rate for the log-concave maximum likelihood estimator given in (1.2.9) when $d = 1, 2$ (up to a logarithmic factor), and since the same entropy integral divergence issues mentioned above apply when $d \geq 4$, we focus on the case $d = 3$ in these sections. In Section 2.3, we restrict attention to densities with polytopal support (that need not satisfy the log-k-affine condition of Section 2.2). Theorem 2.3.1 therein provides a sharp oracle inequality, which reveals that in such cases, the log-concave maximum likelihood estimator attains the rate $\tilde{O}(n^{-4/7})$ with respect to d_X^2 divergence, at least when the density is bounded away from zero on its support.

In Section 2.4, we introduce an alternative way to exclude the bad uniform densities mentioned above, namely by considering subclasses of $\mathcal{F}_d$ consisting of densities f whose contours are well-separated in regions where f is small. A major advantage of working with contour separation, as opposed to imposing a conventional smoothness condition such as Hölder regularity, is that we are able to exhibit adaptation over much wider classes of densities, as we illustrate through several examples in Section 2.4. A consequence of our main theorem in this section (Theorem 2.4.3) is that the log-concave maximum likelihood estimator attains the rate $\tilde{O}(n^{-4/7})$ with respect to d_X^2 divergence over the class of Gaussian densities; again, one can think of this result as partially restoring the original conjecture of Seregin and Wellner (2010), in that their rate is achieved with additional restrictions on the class of log-concave densities. A key feature of our definition of contour separation is that it is affine invariant; since the log-concave maximum likelihood estimator is affine equivariant and our loss functions are affine invariant, this allows us to obtain rates that are uniform over classes without any scale restrictions.

We mention that alternative estimators have also been studied for the class of log-concave densities. One such is the smoothed log-concave maximum likelihood estimator (Chen and Samworth, 2013; Dümbgen and Rufibach, 2009), which matches the first two moments of the empirical distribution of the data, but for which results on rates of convergence are less developed. Another proposal is the

ρ-estimation framework of Baraud and Birgé (2016), for which similar adaptation properties as for the log-concave maximum likelihood estimator are known in the univariate case.

Proofs of most of our main results are given in Section 2.5. The remaining proofs, as well as numerous auxiliary results, are presented in Sections 2.6–2.8.

2.1.1 Notation and background

Recall the expressions for the Hellinger distance d_{H} and Kullback–Leibler divergence KL from (1.2.4) and (1.2.8) respectively. In addition to the notation and concepts in Section 1.4, we make the following definitions. Let $\Phi \equiv \Phi_d$ be the set of all upper semi-continuous, concave functions $\phi\colon \mathbb{R}^d \to [-\infty, \infty)$ and let $\mathcal{G} \equiv \mathcal{G}_d := \{e^{\phi} : \phi \in \Phi\}$. For $\phi \in \Phi$, we write $\operatorname{dom}\phi := \{x \in \mathbb{R}^d : \phi(x) > -\infty\}$ for the *effective domain* of ϕ, and for a general $f\colon \mathbb{R}^d \to \mathbb{R}$, we write $\operatorname{supp} f := \{x \in \mathbb{R}^d : f(x) \neq 0\}$ for the *support* of f. For $k \in \mathbb{N}$, we say that $f \in \mathcal{G}_d$ is *log-k-affine* if there exist closed sets $E_1, \ldots, E_k$ such that $\operatorname{supp} f = \bigcup_{j=1}^{k} E_j$ and $\log f$ is affine on each E_j. Moreover, let $\mathcal{F} \equiv \mathcal{F}_d$ be the family of all *densities* $f \in \mathcal{G}_d$, and let $\mu_f := \int_{\mathbb{R}^d} x f(x)\,dx$ and $\Sigma_f := \int_{\mathbb{R}^d} (x - \mu_f)(x - \mu_f)^\top dx$ for each $f \in \mathcal{F}_d$. In addition, we write $\mathcal{F}^{0,I} \equiv \mathcal{F}_d^{0,I} := \{f \in \mathcal{F}_d : \mu_f = 0,\, \Sigma_f = I\}$ for the class of *isotropic* log-concave densities.

Henceforth, for real-valued functions a and b, we write $a \lesssim b$ if there exists a universal constant $C > 0$ such that $a \leq Cb$, and we write $a \asymp b$ if $a \lesssim b$ and $b \lesssim a$. More generally, for a finite number of parameters $\alpha_1, \ldots, \alpha_r$, we write $a \lesssim_{\alpha_1,\ldots,\alpha_r} b$ if there exists $C \equiv C_{\alpha_1,\ldots,\alpha_r} > 0$, depending only on $\alpha_1, \ldots, \alpha_r$, such that $a \leq Cb$. Also, for $x \in \mathbb{R}$, we write $x^+ := x \vee 0$ and $x^- := (-x)^+$, and for $x > 0$, we define $\log_+ x := 1 \vee \log x$.

To facilitate the exposition in Section 2.4, we introduce some additional terminology. We say that the densities f and g on $\mathbb{R}^d$ are *affinely equivalent* if there exist an $\mathbb{R}^d$-valued random variable X and an invertible affine transformation $T\colon \mathbb{R}^d \to \mathbb{R}^d$ such that X has density f and $T(X)$ has density g; in other words, there exist $b \in \mathbb{R}^d$ and an invertible $A \in \mathbb{R}^{d\times d}$ such that $g(x) = |\det A|^{-1} f\bigl(A^{-1}(x - b)\bigr)$ for all $x \in \mathbb{R}^d$. Thus, each $f \in \mathcal{F}_d$ is affinely equivalent to a unique $f_0 \in \mathcal{F}_d^{0,I}$. A class $\mathcal{D}$ of densities is said to be *affine invariant* if it is closed under affine equivalence; in other words, if f belongs to $\mathcal{D}$, then so does every density g that is affinely equivalent to f.

2.2 Adaptation to log-k-affine densities with polyhedral support

In order to present the main result of this section, we first need to understand the structure of log-k-affine functions $f \in \mathcal{G}_d$ with polyhedral support. Due to the global nature of the constraints on f, namely that $\log f$ is concave on $\operatorname{supp} f \in \mathcal{P}$ and affine on each of k closed subdomains, the function f necessarily has a simple and rigid structure. More precisely, Proposition 2.2.1 below shows that there is a minimal representation of f in which the subdomains are polyhedral sets that form a subdivision of $\operatorname{supp} f$, and the restrictions of $\log f$ to these sets are distinct affine functions. The proof of this result is deferred to Section 2.7.1.

Proposition 2.2.1. *Suppose that $f \in \mathcal{G}_d$ is log-k-affine for some $k \in \mathbb{N}$ and that $\operatorname{supp} f \in \mathcal{P}$. Then there exist $\kappa(f) \leq k$, $\alpha_1, \ldots, \alpha_{\kappa(f)} \in \mathbb{R}^d$, $\beta_1, \ldots, \beta_{\kappa(f)} \in \mathbb{R}$ and a polyhedral subdivision $E_1, \ldots, E_{\kappa(f)}$ of $\operatorname{supp} f$ such that $f(x) = \exp(\alpha_j^\top x + \beta_j)$ for all $x \in E_j$, and $\alpha_i \neq \alpha_j$ whenever $i \neq j$. Moreover, the triples $(\alpha_j, \beta_j, E_j)_{j=1}^{\kappa(f)}$ are unique up to reordering. In addition, if $\operatorname{supp} f \in \mathcal{P}^m$, then $E_j \in \mathcal{P}^{k+m-1}$ for all j.*

In particular, for each such f, the sum of the numbers of facets of the polyhedral subdomains $E_1, \ldots, E_{\kappa(f)}$, which we denote by

$$\Gamma(f) := \sum_{j=1}^{\kappa(f)} |\mathcal{F}(E_j)|, \tag{2.2.1}$$

is well-defined and can be viewed as a parameter that measures the complexity of f. Now for $k \in \mathbb{N}$ and $P \in \mathcal{P}$, let $\mathcal{F}^k(P)$ denote the collection of all $f \in \mathcal{F}_d$ for which $\kappa(f) \leq k$ and $\operatorname{supp} f = P$, so that $\mathcal{F}^k(\mathcal{P}^m) = \bigcup_{P \in \mathcal{P}^m} \mathcal{F}^k(P)$ for $m \in \mathbb{N}_0$. It is shown in Proposition 2.7.10 that $\mathcal{F}^k(\mathcal{P}^m)$ is non-empty if and only if $k + m \geq d + 1$. We remark here that it is more appropriate to quantify the complexity of a polyhedral support in terms of m, which refers to the number of facets of the support, rather than in terms of the number of vertices. Indeed, the former quantity may be much greater than the latter when the support is unbounded; for example, a polyhedral convex cone has just a single vertex but may have arbitrarily many facets. That said, if the support is a polytope with v vertices and m facets, it can be shown that $v = m$ when $d = 2$, and that $v \leq 2m - 4$ and $m \leq 2v - 4$ when $d = 3$; see the proof of Lemma 2.7.12 and the subsequent remark.

We are now in a position to state our sharp oracle inequality for the risk of the log-concave maximum likelihood estimator when the true $f_0 \in \mathcal{F}_d$ is close to some element of $\mathcal{F}^k(\mathcal{P}^m)$.

Theorem 2.2.2. *Fix $d \in \{2, 3\}$. Let $X_1, \ldots, X_n \overset{\mathrm{iid}}{\sim} f_0 \in \mathcal{F}_d$ with $n \geq d + 1$, and let $\hat{f}_n$ denote the corresponding log-concave maximum likelihood estimator. Then there exists a universal constant $C > 0$ such that*

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq \inf_{\substack{k \in \mathbb{N},\, m \in \mathbb{N}_0: \\ k+m \geq d+1}} \inf_{f \in \mathcal{F}^k(\mathcal{P}^m)} \biggl\{ \frac{C\,\Gamma(f)}{n} \log^{\gamma_d} n + \mathrm{KL}(f_0, f) \biggr\}, \tag{2.2.2}$$

where $\gamma_2 := 9/2$ and $\gamma_3 := 8$. Moreover, for $d \in \{2, 3\}$, we have $\Gamma(f) \lesssim k^{d-2}(k + m)$ for all $f \in \mathcal{F}^k(\mathcal{P}^m)$.

The 'sharpness' in this oracle inequality refers to the fact that the approximation term $\mathrm{KL}(f_0, f)$ has leading constant 1. A consequence of Theorem 2.2.2 is that if $d = 2$ and $f_0 \in \mathcal{F}^k(\mathcal{P}^m)$ with $k + m$ small by comparison with $n^{1/3} \log^{-7/2} n$, then the log-concave maximum likelihood estimator attains an adaptive rate that is faster than the rate of decay of the worst-case risk bounds (1.2.9) of Kim and Samworth (2016). When $d = 3$, the same conclusion holds when $k(k + m)$ is small by comparison with $n^{1/2} \log^{-7} n$.

Theorem 2.2.2 is proved in Section 2.5.1 by first considering the case $k = 1$, where it turns out that we can prove a slightly stronger version of our result. We therefore state it separately for convenience:

Theorem 2.2.3. *Fix $d \in \{2, 3\}$. Let $X_1, \ldots, X_n \overset{\mathrm{iid}}{\sim} f_0 \in \mathcal{F}_d$ with $n \geq d + 1$, and let $\hat{f}_n$ denote the corresponding log-concave maximum likelihood estimator. Then there exists a universal constant $\bar{C} > 0$ such that*

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq \inf_{m \geq d} \biggl\{ \frac{\bar{C}m}{n} \log^{\gamma_d} n + \inf_{\substack{f \in \mathcal{F}^1(\mathcal{P}^m) \\ \operatorname{supp} f_0 \subseteq \operatorname{supp} f}} d_{\mathrm{H}}^2(f_0, f) \biggr\}. \tag{2.2.3}$$

We suspect that the restriction on the support of the approximating density f in (2.2.3) is an artefact of our proof. Indeed, in the case $d = 1$, Baraud and Birgé (2016) obtain an oracle inequality for their ρ-estimator where the approximating density f need not have this property (although their result is stated for d_{H}^2 rather than d_X^2); moreover, we have been able to strengthen the corresponding univariate result for the log-concave maximum likelihood estimator (Kim et al., 2018, Theorem 5) by removing this restriction.

The proof of Theorem 2.2.3 in fact constitutes the main technical challenge in deriving Theorem 2.2.2. This entails deriving upper bounds on the (local) Hellinger bracketing entropies of classes of log-concave functions that lie in small Hellinger neighbourhoods of densities in $f \in \mathcal{F}^1(\mathcal{P}^m)$ for each $m \in \mathbb{N}$ with $m \geq d$. Our argument proceeds via a series of steps, the first of which deals with the case where f is a uniform density on a simplex (Proposition 2.6.8); it turns out that any density in a small Hellinger ball around such an f satisfies a uniform upper bound (Lemma 2.7.14(ii)), and a pointwise lower bound whose contours are characterised geometrically in Lemma 2.7.19 (and illustrated in Figure 2.5). We proceed by considering a finite nested sequence of polytopal subsets of the simplex, each of which has a controlled number of vertices and approximates the region enclosed by one of the aforementioned contours; see the accompanying Figure 2.1. After constructing suitable triangulations of the regions between successive polytopes (Corollary 2.7.22), we exploit existing bracketing entropy results for classes of bounded log-concave functions (Proposition 2.6.7).

In the next step, we consider the uniform density on a polytope in $\mathcal{P}^m$; here, using the fact that there is a triangulation of the support into $O(m)$ simplices (Lemma 2.7.12), we apply our earlier bracketing entropy bounds in conjunction with an additional argument which handles carefully the fact that these simplices may have very different volumes (Proposition 2.6.9).

Finally, in the proof of Proposition 2.5.1 in Section 2.5.1, we generalise to settings where f is an arbitrary (not necessarily uniform) log-affine density whose polyhedral support may be unbounded. There, we subdivide the domain by intersecting it with a sequence of parallel half-spaces whose normal vectors are in the direction of the negative log-gradient of the density. Our characterisation of such log-affine densities in Section 2.7.1 ultimately allows us to apply our earlier results to transformations of the original density and thereby obtain the desired local bracketing entropy bounds (Proposition 2.5.1). The conclusion of Theorem 2.2.3 then follows from standard empirical process theory arguments (e.g. van de Geer, 2000, Corollary 7.5); see Section 2.5.1.

We do not claim any optimality of the polylogarithmic factors in Theorems 2.2.2 and 2.2.3. In fact, we can improve these exponents in the special case where f_0 is well-approximated by a uniform density $f_P := \mu_d(P)^{-1}\mathbb{1}_P$ on a polytope $P \in \mathcal{P} \equiv \mathcal{P}_d$. Note that every polytope in $\mathcal{P}_d$ has at least as many facets as a d-simplex, namely $d+1$; see for example Lemma 2.7.11.

Proposition 2.2.4. *Fix $d \in \{2,3\}$, and for $m \geq d+1$, denote by $\mathcal{F}^{[1]}(\mathcal{P}^m)$ the subclass of all uniform densities on polytopes in $\mathcal{P}^m$. Let $X_1,\ldots,X_n \overset{\mathrm{iid}}{\sim} f_0 \in \mathcal{F}_d$ with $n \geq d+1$, and let $\hat{f}_n$ denote the corresponding log-concave maximum likelihood estimator. Then there exists a universal constant $C' > 0$ such that*

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq \inf_{m \geq d+1} \biggl\{\frac{C'm}{n}\log^{\gamma_d'} n + \inf_{\substack{f \in \mathcal{F}^{[1]}(\mathcal{P}^m) \\ \mathrm{supp}\, f_0 \subseteq \mathrm{supp}\, f}} d_{\mathrm{H}}^2(f_0, f)\biggr\}, \tag{2.2.4}$$

where $\gamma_2' := 3$ and $\gamma_3' := 6$.

2.3 Adaptation to densities bounded away from zero on a polytopal support

Recall from the discussion in the introduction that in order to observe adaptive behaviour for the log-concave maximum likelihood estimator, we need to exclude uniform densities supported on convex sets with smooth boundaries. In fact, we will see from Proposition 2.3.2 below that we also need to rule out subclasses containing sequences of elements of $\mathcal{F}_d$ that approximate such uniform densities. In this section, we continue to work with densities in $\mathcal{F}_d$ that are close to a log-concave density with polyhedral support, but, in contrast to Section 2.2, now drop the requirement that this approximating density be log-k-affine. In fact, we do not impose any extra structural constraints or smoothness conditions that would regulate further the behaviour of the densities on the interiors of their supports. It will turn out, however, that we will only be able to improve on the worst-case risk bounds of Theorem 2.6.2 when the approximating density is also bounded away from zero on its support, which must therefore necessarily be a polytope. The generality of the resulting new classes means that we can no longer expect near-parametric adaptation, and moreover, for the reasons explained in the introduction, our main result of this section (Theorem 2.3.1 below) is restricted to the case $d = 3$. As an example of a density that will be covered by this result, we can consider the density of a trivariate Gaussian random vector conditioned to lie in $[-1, 1]^3$.

The proofs of both results in this section are given in Section 2.5.2.

Following on from Proposition 2.2.4, we now extend the definition of $\mathcal{F}^{[1]}(\mathcal{P}^m)$ given above and introduce our new family of subclasses of $\mathcal{F}_d$. For $\theta \in (0, \infty)$ and a polytope $P \in \mathcal{P}_d$, let $\mathcal{F}^{[\theta]}(P) \equiv \mathcal{F}_d^{[\theta]}(P)$ denote the collection of all $f \in \mathcal{F}_d$ for which $\operatorname{supp} f = P$ and $f \geq \theta^{-1} f_P$ on P. Then $\mathcal{F}^{[1]}(P) = \{f_P\}$ and $\mathcal{F}^{[\theta]}(P)$ is non-empty if and only if $\theta \geq 1$. For $\theta \in [1, \infty)$ and $m \in \mathbb{N}$ with $m \geq d + 1$, denote by $\mathcal{F}^{[\theta]}(\mathcal{P}^m) \equiv \mathcal{F}_d^{[\theta]}(\mathcal{P}_d^m)$ the union of those $\mathcal{F}^{[\theta]}(P)$ for which P is a polytope in $\mathcal{P}^m \equiv \mathcal{P}_d^m$, and note that this is a non-empty affine invariant subclass of $\mathcal{F}_d$. Indeed, fix $b \in \mathbb{R}^d$ and an invertible $A \in \mathbb{R}^{d \times d}$, and let $T \colon \mathbb{R}^d \to \mathbb{R}^d$ be the invertible affine transformation defined by $T(x) := Ax + b$. If $X \sim f \in \mathcal{F}^{[\theta]}(P)$ for some polytope $P \in \mathcal{P}^m$, then $\mu_d(T(P)) = |\det A| \, \mu_d(P)$, and so the density g of $T(X)$ satisfies $g(x) = |\det A|^{-1} f(T^{-1}(x)) \geq \{\theta \, |\det A| \, \mu_d(P)\}^{-1} = \{\theta \mu_d(T(P))\}^{-1}$ for all $x \in T(P)$. Since $\operatorname{supp} g = T(P)$ is also a polytope in $\mathcal{P}^m$, this shows that $g \in \mathcal{F}^{[\theta]}(\mathcal{P}^m)$, as required.

The sharp oracle inequality (2.3.1) below may be viewed as complementary to Theorem 2.2.3 and Proposition 2.2.4.

Theorem 2.3.1. *Let $X_1, \ldots, X_n \overset{\mathrm{iid}}{\sim} f_0 \in \mathcal{F}_3$ with $n \geq 4$, and let $\hat{f}_n$ denote the corresponding log-concave maximum likelihood estimator. Then there exists a universal constant $C > 0$ such that*

$$\begin{aligned} &\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \\ &\leq \inf_{\substack{m \geq 4 \\ \theta \in (1,\infty)}} \biggl\{ C \biggl(\log^{6/7} \theta \, \Bigl(\frac{m}{n}\Bigr)^{4/7} \log_+^{17/7} \Bigl(\frac{n}{\log^{3/2} \theta}\Bigr) + \Bigl(\frac{m}{n}\Bigr)^{20/29} \log^{85/29} n + \theta \log^3(e\theta) \, \frac{m \log^6 n}{n} \biggr) \\ &\qquad\qquad + \inf_{\substack{f \in \mathcal{F}_3^{[\theta]}(\mathcal{P}^m) \\ \operatorname{supp} f_0 \subseteq \operatorname{supp} f}} d_{\mathrm{H}}^2(f_0, f) \biggr\}. \end{aligned} \tag{2.3.1}$$

For a fixed $\theta \in (1, \infty)$, note that if n/m is sufficiently large, then the dominant contribution to the right hand side of (2.3.1) comes from the first term. It follows that for fixed θ, m, the log-concave maximum likelihood estimator $\hat{f}_n$ of $f_0 \in \mathcal{F}_3^{[\theta]}(\mathcal{P}^m)$ converges at rate $\tilde{O}(n^{-4/7})$ as $n \to \infty$, which was the rate originally conjectured by Seregin and Wellner (2010).

Despite the attractions of the adaptation mentioned in the previous paragraph, it is worth considering the bound (2.3.1) in the limits as $\theta \searrow 1$ and $\theta \to \infty$. In the first case, owing to the presence of the second term on the right hand side of (2.3.1), we do not recover the bound (2.2.4) from Proposition 2.2.4 when we take the limit of the right hand side of (2.3.1); see Section 2.6.3 for further discussion. We also mention here that for a fixed n, the bound in (2.2.4) may be stronger than that in (2.3.1) if for example $f_0 \in \mathcal{F}_3^{[\theta]}(\mathcal{P}^m)$ for some $\theta \equiv \theta_n \in (1, \infty)$ sufficiently close to 1. To substantiate this remark, we note that if $\theta \in [1, \infty)$ and $P \in \mathcal{P}_3$ is a polytope, then it follows from the proof of Lemma 2.7.14(iii) that every $f \in \mathcal{F}_3^{[\theta]}(P)$ satisfies $\theta^{-1} f_P \leq f \lesssim \log^3(e\theta) f_P$ on P. Thus, if $f_0 \in \mathcal{F}_3^{[\theta]}(P)$, then

$$d_{\mathrm{H}}^2(f_0, f_P) = \int_P \bigl(\sqrt{f_0} - \sqrt{f_P}\bigr)^2 \lesssim (1-\theta^{-1}) \vee \bigl(\log^3(e\theta) - 1\bigr) \lesssim \theta - 1$$

when $\theta \leq 2$. Consequently, if n is fixed and θ, m are such that $\theta \leq 1 + n^{-20/29}$ and $m \leq n^{9/29} \log^{-6} n$, then for any $f_0 \in \mathcal{F}_3^{[\theta]}(P)$ with $P \in \mathcal{P}^m$, the bound in (2.2.4) is at most a universal constant multiple of $(m/n)\log^6 n + (\theta - 1) \lesssim n^{-20/29}$, whereas the bound in (2.3.1) is at least a universal constant multiple of $n^{-20/29} \log^{85/29} n$.

It is also notable that the bound in (2.3.1) diverges to infinity as $\theta \to \infty$. In fact, we will deduce from Proposition 2.3.2 below that this is not just an artefact of our analysis; more precisely, the log-concave maximum likelihood estimator does not adapt uniformly over $\bigcup_{\theta \geq 1} \mathcal{F}_d^{[\theta]}(P)$, or indeed over any subclass of $\mathcal{F}_d$ containing an approximating sequence for a uniform density on a closed Euclidean ball.

Proposition 2.3.2. *Fix $d \in \mathbb{N}$ and $n \geq d+1$. Let $(f^{(\ell)})$ be a sequence of densities in $\mathcal{F}_d$ for which the corresponding sequence of probability measures $(P^{(\ell)})$ converges weakly to a distribution $P^{(0)}$ with density $f^{(0)} \colon \mathbb{R}^d \to [0,\infty)$. For each $\ell \in \mathbb{N}_0$, let $X_1^{(\ell)}, \ldots, X_n^{(\ell)} \overset{\mathrm{iid}}{\sim} f^{(\ell)}$, and let $\hat{f}_n^{(\ell)}$ denote the corresponding log-concave maximum likelihood estimator. Then*

$$\liminf_{\ell \to \infty} \mathbb{E}\bigl\{d_X^2\bigl(\hat{f}_n^{(\ell)}, f^{(\ell)}\bigr)\bigr\} \geq \mathbb{E}\bigl\{d_X^2\bigl(\hat{f}_n^{(0)}, f^{(0)}\bigr)\bigr\}.$$

To understand the consequences of this lower semi-continuity result, fix any polytope $P \in \mathcal{P}_d$ and a closed Euclidean ball $B \subseteq \operatorname{Int} P$. We can find a sequence $(f^{(\ell)})$ in $\bigcup_{\theta \geq 1} \mathcal{F}_d^{[\theta]}(P)$ such that the corresponding probability measures converge weakly to the uniform distribution on B. Such a sequence must necessarily satisfy $\inf_{x \in P} f^{(\ell)}(x) \to 0$, and Proposition 2.3.2, together with the result of Wieacker (1987) mentioned in the introduction, then ensures that $\liminf_{\ell \to \infty} \mathbb{E}\bigl\{d_X^2\bigl(\hat{f}_n^{(\ell)}, f^{(\ell)}\bigr)\bigr\} \gtrsim_d n^{-2/(d+1)}$ for $d \geq 2$. Thus, indeed, no adaptation is possible.

The proof of Theorem 2.3.1 follows a similar approach to that set out after the statement of Theorem 2.2.3. The key intermediate results are the local bracketing entropy bounds in Propositions 2.6.10 and 2.6.11 in Section 2.6.3, which are analogous to the Propositions 2.6.8 and 2.6.9 that prepare the ground for the proof of Theorem 2.2.3. As we explain in the discussion before the proof of Proposition 2.6.8, some modifications to the previous arguments are necessary, but we once again draw heavily on the technical apparatus developed in Section 2.7.2. The key reason we are able to apply these techniques here is that the densities in $\mathcal{F}^{[\theta]}(\mathcal{P}^m)$ are bounded away from zero, as evidenced by the fact that the bound (2.3.1) diverges as $\theta \to \infty$. Once we have obtained Proposition 2.6.11, all that remains is to appeal to standard empirical process theory (van de Geer, 2000, Corollary 7.5), from which the desired conclusion (2.3.1) follows readily; see Section 2.5.2. In contrast to the proof of Theorem 2.2.3, we do not require an additional argument along the lines of the proof of Proposition 2.5.1 given in Section 2.5.1, which is specific to the log-1-affine densities (with possibly unbounded polyhedral support) studied in Section 2.2.

2.4 Adaptation to densities with well-separated contours

In this section, we consider adaptation of the log-concave maximum likelihood estimator over yet further subclasses of $\mathcal{F}_d$. As discussed in Examples 2.4 and 2.5 below, these are designed to generalise notions of Hölder smoothness, while at the same time satisfying our key property of affine invariance. Given $S \in \mathbb{S}^{d \times d}$ and $x \in \mathbb{R}^d$, we write $\|x\|_S := (x^\top S^{-1} x)^{1/2}$ for its *S-Mahalanobis norm*.

Definition 1. *For $\beta \geq 1$ and $\Lambda, \tau > 0$, let $\mathcal{F}^{(\beta,\Lambda,\tau)} \equiv \mathcal{F}_d^{(\beta,\Lambda,\tau)}$ denote the collection of all $f \in \mathcal{F}_d$ that are continuous on $\mathbb{R}^d$ and satisfy*

$$\|x-y\|_{\Sigma_f} \geq \frac{\{f(x)-f(y)\}\det^{1/2}\Sigma_f}{\Lambda\left\{f(x)\det^{1/2}\Sigma_f\right\}^{1-1/\beta}} \tag{2.4.1}$$

whenever $x, y \in \mathbb{R}^d$ are such that $f(y) < f(x) < \tau\det^{-1/2}\Sigma_f$. In addition, we define $\mathcal{F}^{(\beta,\Lambda)} := \bigcap_{\tau>0}\mathcal{F}^{(\beta,\Lambda,\tau)}$.

The defining condition (2.4.1) imposes a separation condition on contours below some fixed level. For instance, when f is isotropic, the condition asks that for all small $t > 0$, the contours of f at levels t and $2t$ are at least a distance of order $\Lambda^{-1}t^{1/\beta}$ apart. See below for further discussion and motivating examples. We now collect together some basic properties of the classes $\mathcal{F}^{(\beta,\Lambda,\tau)}$.

Proposition 2.4.1. *For $\beta \geq 1$ and $\Lambda, \tau > 0$, we have the following:*

(i) $\mathcal{F}^{(\beta,\Lambda,\tau)}$ *is* affine invariant*; i.e. if $X \sim f \in \mathcal{F}^{(\beta,\Lambda,\tau)}$ and $T\colon \mathbb{R}^d \to \mathbb{R}^d$ is an invertible affine transformation, then the density g of $T(X)$ also lies in $\mathcal{F}^{(\beta,\Lambda,\tau)}$.*

(ii) $\mathcal{F}^{(\beta,\Lambda,\tau)} \subseteq \mathcal{F}^{(\beta,\Lambda^*)}$ *for all $\Lambda^* \geq \Lambda(B_d/\tau)^{1/\beta}$, where $B_d := \sup_{h\in\mathcal{F}_d^{0,I}}\sup_{x\in\mathbb{R}^d} h(x) \in (0,\infty)$.*

(iii) If $\alpha \in [1,\beta)$, then $\mathcal{F}^{(\beta,\Lambda,\tau)} \subseteq \mathcal{F}^{(\alpha,\Lambda',\tau)}$ for all $\Lambda' \geq B_d^{1/\alpha-1/\beta}\Lambda$.

(iv) There exists $\Lambda_{0,d} > 0$, depending only on d, such that $\mathcal{F}^{(\beta,\Lambda)}$ is non-empty only if $\Lambda \geq \Lambda_{0,d}$.

Note in particular that since the log-concave maximum likelihood estimator $\hat{f}_n$ is affine equivariant (Dümbgen et al., 2011, Remark 2.4), and since our loss functions d_{H}^2, KL and d_X^2 are affine invariant, property (i) above allows us to restrict attention to *isotropic* $f \in \mathcal{F}^{(\beta,\Lambda,\tau)}$, namely those belonging to $\mathcal{F}_d^{0,I}$. Property (iii) indicates that the classes $\mathcal{F}^{(\beta,\Lambda,\tau)}$ are nested with respect to the exponent $\beta \geq 1$.

In addition, by taking $\alpha = 1$ in (iii) and then applying (ii), we deduce that the densities in $\mathcal{F}^{(\beta,\Lambda,\tau)}$ are all Lipschitz on $\mathbb{R}^d$, but as we will see in Examples 2.2 and 2.4, they need not be differentiable everywhere. In cases where $f \in \mathcal{F}_d$ is differentiable on an open set of the form $\{x \in \mathbb{R}^d : f(x) < \tau^*\}$ for some $\tau^* > 0$, the necessary and sufficient condition in the following proposition provides us with a simpler way of checking whether f lies in $\mathcal{F}^{(\beta,\Lambda,\tau)}$. For $w \in \mathbb{R}^d$ and $S \in \mathbb{S}^{d\times d}$, let $\|w\|_S' := (w^\top S^{-1}w)^{1/2}\det^{-1/2}S$ denote its *scaled S-Mahalanobis norm*.

Proposition 2.4.2. *Suppose that there exists $\tau^* > 0$ such that $f \in \mathcal{F}_d$ is continuous on $\mathbb{R}^d$ and differentiable at every $x \in \mathbb{R}^d$ satisfying $f(x) < \tau^*$. Then for $\beta \geq 1$ and any $\tau \leq \tau^*\det^{1/2}\Sigma_f$, we have $f \in \mathcal{F}^{(\beta,\Lambda,\tau)}$ if and only if*

$$\|\nabla f(x)\|_{\Sigma_f^{-1}}' \leq \Lambda\left\{f(x)\det^{1/2}\Sigma_f\right\}^{1-1/\beta} \tag{2.4.2}$$

for all $x \in \mathbb{R}^d$ with $f(x) < \tau\det^{-1/2}\Sigma_f$.

Our main result in this section is a sharp oracle inequality for the performance of the log-concave maximum likelihood estimator when the true log-concave density is close to $\mathcal{F}_d^{(\beta,\Lambda)}$ when $d = 3$. In view of Proposition 2.4.1(ii), we work here with the classes $\mathcal{F}_3^{(\beta,\Lambda)}$ rather than the more general classes $\mathcal{F}_3^{(\beta,\Lambda,\tau)}$ for ease of presentation. Let $\Lambda_0 \equiv \Lambda_{0,3} > 0$ be the universal constant from Proposition 2.4.1(iv) and its proof, and for each $\beta \geq 1$, let $r_\beta := \frac{\beta+3}{\beta+7} \wedge \frac{4}{7}$.

Theorem 2.4.3. *Let $X_1, \ldots, X_n \overset{\mathrm{iid}}{\sim} f_0 \in \mathcal{F}_3$ for some $n \geq 4$, and let $\hat{f}_n$ denote the corresponding log-concave maximum likelihood estimator. Then there exists a universal constant $C > 0$ such that*

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq \inf_{\beta\geq 1,\,\Lambda\geq\Lambda_0}\left\{C\Lambda^{\frac{4\beta}{\beta+7}\wedge 1}n^{-r_\beta}\log^{\frac{16\beta+39}{2(\beta+3)}r_\beta} n + \inf_{f\in\mathcal{F}_3^{(\beta,\Lambda)}} d_{\mathrm{H}}^2(f_0, f)\right\}. \tag{2.4.3}$$

Ignoring polylogarithmic factors and focusing on the case where $f_0 \in \mathcal{F}_3^{(\beta,\Lambda)}$ for some $\beta \geq 1$ and $\Lambda > 0$, Theorem 2.4.3 presents a continuum of rates that interpolate between the worst-case rate of $\tilde{O}(n^{-1/2})$, corresponding to the rate when $\beta = 1$, and $\tilde{O}(n^{-4/7})$, again matching the rate conjectured by Seregin and Wellner (2010).

The proofs of all results in this section are given in Section 2.5.3.

As mentioned in the introduction, the main attraction of working with the general contour separation condition (2.4.1) is that we can give several examples of classes of densities contained within $\mathcal{F}^{(\beta,\Lambda,\tau)}$ for suitable β, Λ and τ. Since each of the conditions (2.4.1) and (2.4.2) are affine invariant, it suffices to check these conditions for the isotropic elements of the relevant classes (or for any other convenient choice of scaling). Moreover, to verify (2.4.1) for densities that are spherically symmetric, it suffices to consider pairs x, y of the form $y = \lambda x$ for some $\lambda > 0$; in other words, if $f(x) = g(\|x\|)$, then it is enough to verify the contour separation condition (2.4.1) for g.

Example 2.1 (Gaussian densities)**.** Writing $f\colon x \mapsto (2\pi)^{-d/2}\, e^{-\|x\|^2/2}$ for the standard Gaussian density on $\mathbb{R}^d$ and fixing an arbitrary $\beta \geq 1$, we have

$$\|\nabla f(x)\|_I' = \|\nabla f(x)\| = \frac{\|x\|}{(2\pi)^{d/2}}\, e^{-\|x\|^2/2} = 2^{1/2} f(x) \log^{1/2}\biggl(\frac{1}{(2\pi)^{d/2} f(x)}\biggr)$$
$$\leq \frac{\beta^{1/2}}{(2\pi)^{d/(2\beta)}}\, e^{-1/2} f(x)^{1-1/\beta}$$

for all $x \in \mathbb{R}^d$. Hence, it follows from Proposition 2.4.2 that $f \in \mathcal{F}^{(\beta,\Lambda)}$ for all $\beta \geq 1$, with $\Lambda = \beta^{1/2} e^{-1/2}\, (2\pi)^{-d/(2\beta)}$. Thus, Theorem 2.4.3 implies that when $d = 3$, the log-concave maximum likelihood estimator attains the rate $\tilde{O}(n^{-4/7})$ in d_X^2 divergence uniformly over the class of Gaussian densities.

Example 2.2 (Spherically symmetric Laplace density)**.** Let $V_d := \mu_d(\bar{B}(0,1)) = \pi^{d/2}/\Gamma(1 + d/2)$. Then $f\colon x \mapsto (d!\, V_d)^{-1} e^{-\|x\|}$ is a density in $\mathcal{F}_d$ with corresponding covariance matrix $\Sigma \equiv \Sigma_f = (d+1)I$. For $\tau \leq (d+1)^{d/2}\, (d!\, V_d)^{-1}$ and any $\beta \geq 1$, we have

$$\|\nabla f(x)\|_{\Sigma^{-1}}' = (d+1)^{(d+1)/2} f(x) \leq \frac{(d+1)^{(d+1)/2}}{(d!\, V_d)^{1/\beta}} f(x)^{1-1/\beta}$$

for all $x \in \mathbb{R}^d$ with $f(x) < \tau \det^{-1/2}\Sigma = \tau(d+1)^{-d/2}$. Hence, when $d = 3$, the log-concave maximum likelihood estimator attains the rate $\tilde{O}(n^{-4/7})$ in d_X^2 divergence uniformly over the class of densities that are affinely equivalent to f, even though f is not differentiable at 0. A similar conclusion holds for the densities f_1, f_2 satisfying $f_1(x) \propto \exp(-e^{\|x\|})$ and $f_2(x) \propto \exp\bigl(-e^{e^{\|x\|}}\bigr)$.

Example 2.3 (Spherically symmetric bump function density)**.** Consider the smooth density $f\colon x \mapsto Ce^{-1/(1-\|x\|^2)} \mathbb{1}_{\{\|x\|<1\}}$, where $C > 0$ is a normalisation constant. By Xu and Samworth (2021, Proposition 2), f is log-concave. Writing $\Sigma \equiv \Sigma_f = \sigma^2 I$ for the covariance matrix corresponding to f, and again fixing an arbitrary $\beta \geq 1$, we see that each $x \in \mathbb{R}^d$ with $\|x\| < 1$ satisfies

$$\|\nabla f(x)\|_{\Sigma^{-1}}' = \sigma^{d+1}\|\nabla f(x)\| = \sigma^{d+1} \frac{2C\|x\|}{(1 - \|x\|^2)^2}\, e^{-1/(1-\|x\|^2)}$$
$$\leq 2\sigma^{d+1} f(x) \log^2\biggl(\frac{C}{f(x)}\biggr) \leq \Lambda_\beta \bigl\{f(x) \det^{1/2}\Sigma\bigr\}^{1-1/\beta},$$

where $\Lambda_\beta := 8C^{1/\beta}\beta^2 e^{-2}\sigma^{1+d/\beta}$. Thus, again by Proposition 2.4.2, we deduce that $f \in \mathcal{F}^{(\beta,\Lambda_\beta)}$ for all $\beta \geq 1$. Consequently, when $d = 3$, the log-concave maximum likelihood estimator attains the rate $\tilde{O}(n^{-4/7})$ in d_X^2 divergence uniformly over the class of densities that are affinely equivalent to f.

Example 2.4 (Hölder condition on the log-density)**.** For $\gamma \in (1,2]$ and $L > 0$, let $\tilde{\mathcal{H}}^{\gamma,L} \equiv \tilde{\mathcal{H}}_d^{\gamma,L}$ denote the subset of densities $f \in \mathcal{F}_d$ such that $\phi := \log f$ is differentiable and

$$\|\nabla\phi(y) - \nabla\phi(x)\|_{\Sigma_f^{-1}} \leq L\|y-x\|_{\Sigma_f}^{\gamma-1} \tag{2.4.4}$$

for all $x, y \in \mathbb{R}^d$. We extend this definition to $\gamma = 1$ by writing $\tilde{\mathcal{H}}^{1,L}$ for the subset of densities $f \in \mathcal{F}_d$ for which $\phi = \log f$ satisfies

$$|\phi(y) - \phi(x)| \leq L\|y-x\|_{\Sigma_f}. \tag{2.4.5}$$

for all $x, y \in \mathbb{R}^d$. Note that the densities in $\tilde{\mathcal{H}}^{1,L}$ can have points of non-differentiability for arbitrarily small values of the density. For instance, if we define $f \in \mathcal{F}_d$ by

$$f(x) \propto \exp\biggl(-\sum_{r=0}^{\infty} \frac{\|x\| - r}{2^r}\,\mathbb{1}_{\{\|x\| \geq r\}}\biggr),$$

which is not differentiable at any $x \in \mathbb{R}^d$ with integer Euclidean norm, then $f \in \tilde{\mathcal{H}}^{1,L}$ for suitably large $L > 0$.

The careful and non-standard choice of norms in (2.4.4) and (2.4.5) ensures that the classes $\tilde{\mathcal{H}}^{\gamma,L}$ are affine invariant. Moreover, Proposition 2.8.7(iv) in Section 2.8.1 shows that for each $\beta \geq 1$, there exists $\Lambda' \equiv \Lambda'(\beta, L)$ such that $\bigcup_{\gamma\in[1,2]} \tilde{\mathcal{H}}^{\gamma,L} \subseteq \mathcal{F}^{(\beta,\Lambda')}$. Thus, when $d = 3$, the log-concave maximum likelihood estimator attains the rate $\tilde{O}(n^{-4/7})$ in d_X^2 divergence uniformly over $\bigcup_{\gamma\in[1,2]} \tilde{\mathcal{H}}^{\gamma,L}$.

A related result in the literature is Dümbgen and Rufibach (2009, Theorem 4.1), which applies when $d = 1$, $\gamma \in (1,2]$ and the logarithm of the true fixed $f_0 \in \mathcal{F}_1$ is γ-Hölder on some compact subinterval T of the interior of $\operatorname{supp} f_0$. In this case, the corresponding $\hat{f}_n$ is shown to achieve an adaptive rate of order $\bigl(\frac{\log n}{n}\bigr)^{\frac{\gamma}{2\gamma+1}}$ with respect to the supremum norm over certain compact subintervals of the interior of T. We remark that this is not entirely comparable with the rate we obtain in the paragraph above, especially since our loss function d_X^2 is rather different.

Observe that the densities in the classes $\tilde{\mathcal{H}}^{\gamma,L}$ must be supported on the whole of $\mathbb{R}^d$, and that conditions (2.4.4) and (2.4.5) imply that the rate of tail decay of f is 'super-Gaussian'. This is quite a stringent restriction; note for example that the density f satisfying $f(x) \propto \exp(-e^{\|x\|})$ does not feature in any of the classes $\tilde{\mathcal{H}}^{\gamma,L}$. Another drawback of this definition of smoothness is that the classes are not nested with respect to the Hölder exponent $\gamma \in (1,2]$; this can be seen by considering a density f satisfying $f(x) \propto \exp(-\|x\|^{\gamma})$, which belongs to $\tilde{\mathcal{H}}^{\tilde{\gamma},L}$ for some $L > 0$ if and only if $\tilde{\gamma} = \gamma$.

Example 2.5 (Hölder condition on the density)**.** To remedy the issues mentioned in the previous example, fix $\beta \in (1,2]$ and $L > 0$, and let $\mathcal{H}^{\beta,L} \equiv \mathcal{H}_d^{\beta,L}$ denote the set of $f \in \mathcal{F}_d$ such that f is differentiable on $\mathbb{R}^d$ and

$$\|\nabla f(y) - \nabla f(x)\|'_{\Sigma_f^{-1}} \leq L\|y-x\|_{\Sigma_f}^{\beta-1} \tag{2.4.6}$$

for all $x, y \in \mathbb{R}^d$. Again, it can be shown that the classes $\mathcal{H}^{\beta,L}$ are affine invariant, and if $f \in \mathcal{F}_d$ is β-Hölder in the usual Euclidean sense, i.e. $\|\nabla f(y) - \nabla f(x)\| \leq L\|y-x\|^{\beta-1}$ for all $x, y \in \mathbb{R}^d$, then $f \in \mathcal{H}^{\beta,\tilde{L}}$ with $\tilde{L} := L\,\lambda_{\max}^{\beta/2}(\Sigma_f)\det^{1/2}\Sigma_f$, where $\lambda_{\max}(\Sigma_f)$ denotes the maximum eigenvalue of Σ_f. This is because $\|w\|_{\Sigma_f} \geq \|w\|\,\lambda_{\max}^{-1/2}(\Sigma_f)$ and $\|w\|'_{\Sigma_f^{-1}} \leq \|w\|\,\lambda_{\max}^{1/2}(\Sigma_f)\det^{1/2}\Sigma_f$ for all $w \in \mathbb{R}^d$.

The condition (2.4.6) can in fact be extended to an affine invariant notion of β-Hölder regularity for all $\beta > 1$; see Section 2.8.2 for full technical details. Here, we present the analogue of (2.4.6) for $\beta \in (2,3]$ and $L > 0$, for which we require the following additional notation. First, if $g\colon \mathbb{R}^d \to \mathbb{R}$ is twice differentiable at $x \in \mathbb{R}^d$, then denote by $Hg(x) \in \mathbb{R}^{d\times d}$ the Hessian of g at x. In addition, for each $S \in \mathbb{S}^{d\times d}$, define a norm $\|\cdot\|'_S$ on $\mathbb{R}^{d\times d}$ by $\|M\|'_S := \|S^{-1/2}MS^{-1/2}\|_{\mathrm{F}}\det^{-1/2}S$, where $\|A\|_{\mathrm{F}} := \operatorname{tr}(A^{\top}A)^{1/2}$ denotes the Frobenius norm of $A \in \mathbb{R}^{d\times d}$. We now define $\mathcal{H}^{\beta,L}$ to be the collection of $f \in \mathcal{F}_d$ for which f is twice differentiable on $\mathbb{R}^d$ and

$$\|Hf(y) - Hf(x)\|'_{\Sigma_f^{-1}} \leq L\|y - x\|_{\Sigma_f}^{\beta-2} \tag{2.4.7}$$

for all $x, y \in \mathbb{R}^d$. In Section 2.8.2, we present a unified argument that establishes the affine invariance of the classes $\mathcal{H}^{\beta,L}$ defined by (2.4.6) and (2.4.7); see the proof of Lemma 2.8.5. Moreover, Proposition 2.8.6 shows that the classes $\mathcal{H}^{\beta,L}$ are nested with respect to the Hölder exponent β; more precisely, if $\beta > 1$ and $L > 0$, then there exists $\tilde{L} \equiv \tilde{L}(d, \beta, L) > 0$ such that $\mathcal{H}^{\beta,L} \subseteq \mathcal{H}^{\alpha,\tilde{L}}$ for all $\alpha \in (1, \beta]$.

In addition, for each $\beta \in (1, 3]$ and $L > 0$, parts (i) and (iii) of Proposition 2.8.7 imply that $\mathcal{H}^{\beta,L} \subseteq \mathcal{F}^{(\beta,\Lambda)}$ for some $\Lambda \equiv \Lambda(\beta, L)$; when $\beta \in (1, 2]$, we can take $\Lambda(\beta, L) := L^{1/\beta}(1 - 1/\beta)^{-1+1/\beta}$. It was this fact that motivated our choice of parametrisation in β in (2.4.1). For any $\beta > 3$ and $L > 0$, it follows from Proposition 2.8.6 that there exists $\tilde{L} \equiv \tilde{L}(\beta, L) > 0$ such that $\mathcal{H}^{\beta,L} \subseteq \mathcal{H}^{3,\tilde{L}}$. Theorem 2.4.3 therefore yields the rate $\tilde{O}\bigl(n^{-\min\{\frac{\beta+3}{\beta+7}, \frac{4}{7}\}}\bigr)$ for the log-concave maximum likelihood estimator, uniformly over $\mathcal{H}^{\beta,L}$, for any $\beta > 1$. An interesting feature of this rate is that, when $\beta \in (1, 9/5)$, it is faster than the rate $O(n^{-\frac{2\beta}{2\beta+3}})$ that can be obtained in squared Hellinger distance for β-Hölder densities that satisfy a 'tail dominance' condition (Goldenshluger and Lepski, 2014, Section 4). For further details of this comparison, see Section 2.8.2. Thus, in this range of β, the log-concavity shape constraint results in a strict improvement in the rates attainable.

2.5 Proofs of main results

The following notation is throughout the rest of Chapter 2.

To define bracketing entropy, let $S \subseteq \mathbb{R}^d$ and let $\mathcal{G}$ be a class of non-negative functions whose domains contain S. For $\varepsilon > 0$ and a semi-metric ρ on $\mathcal{G}$, let $N_{[]}(\varepsilon, \mathcal{G}, \rho, S)$ denote the smallest $M \in \mathbb{N}$ for which there exist pairs of functions $\{[g_j^L, g_j^U] : j = 1, \ldots, M\}$ such that $\rho(g_j^U, g_j^L) \leq \varepsilon$ for every $j = 1, \ldots, M$, and such that for every $g \in \mathcal{G}$, there exists $j^* \in \{1, \ldots, M\}$ with $g_{j^*}^L(x) \leq g(x) \leq g_{j^*}^U(x)$ for every $x \in S$. We then define the *ε-bracketing entropy of $\mathcal{G}$ over S with respect to ρ* by $H_{[]}(\varepsilon, \mathcal{G}, \rho, S) := \log N_{[]}(\varepsilon, \mathcal{G}, \rho, S)$ and write $H_{[]}(\varepsilon, \mathcal{G}, \rho) := H_{[]}(\varepsilon, \mathcal{G}, \rho, \mathbb{R}^d)$ when $S = \mathbb{R}^d$.

For each $f_0 \in \mathcal{F}_d$ and $\delta > 0$, let $\mathcal{G}(f_0, \delta) \equiv \mathcal{G}_d(f_0, \delta) := \{f\mathbb{1}_{\mathrm{supp}\, f_0} : f \in \mathcal{G}_d,\ d_{\mathrm{H}}(f, f_0) \leq \delta\}$. In addition, let $\mathcal{F}(f_0, \delta) \equiv \mathcal{F}_d(f_0, \delta) = \mathcal{F}_d \cap \mathcal{G}_d(f_0, \delta)$ and let $\tilde{\mathcal{F}}(f_0, \delta) \equiv \tilde{\mathcal{F}}_d(f_0, \delta) := \{f \in \mathcal{F}_d : d_{\mathrm{H}}(f, f_0) \leq \delta\}$. Writing $\|M\| \equiv \|M\|_{\mathrm{op}} := \sup_{\|u\| \leq 1} \|Mu\|$ for the operator norm of a matrix $M \in \mathbb{R}^{d \times d}$, we denote by $\tilde{\mathcal{F}}^{1,\eta} \equiv \tilde{\mathcal{F}}_d^{1,\eta_d} := \{f \in \mathcal{F}_d : \|\mu_f\| \leq 1, \|\Sigma_f - I\| \leq \eta_d\}$ the class of *'near-isotropic'* log-concave densities, where the constant $\eta \equiv \eta_d \in (0, 1)$ is taken from Kim and Samworth (2016, Lemma 6) and depends only on d. Finally, we define $h_2, h_3 \colon (0, \infty) \to (0, \infty)$ by $h_2(x) := x^{-1} \log_+^{3/2}(x^{-1})$ and $h_3(x) := x^{-2}$ respectively.

2.5.1 Proofs of main results in Section 2.2

The proof of Proposition 2.2.1 is lengthy and is deferred to Section 2.7.1. The main goal of this subsection, therefore, is to prove Theorem 2.2.2, which proceeds via several intermediate results, including Theorem 2.2.3. We begin by stating our main local bracketing entropy result, whose proof is summarised at the end of Section 2.2. Note that by Proposition 2.7.10, the subclass $\mathcal{F}^1(\mathcal{P}^m)$ is non-empty if and only if $m \geq d$.

Proposition 2.5.1. *Let $d \in \{2, 3\}$ and fix $m \in \mathbb{N}$ with $m \geq d$. Then there exist universal constants $\varrho_2, \varrho_3 > 0$ such that whenever $0 < \varepsilon < \delta < \varrho_d$ and $f_0 \in \mathcal{F}^1(\mathcal{P}^m)$, we have*

$$H_{[]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0, \delta), d_{\mathrm{H}}\bigr) \lesssim m\left(\frac{\delta}{\varepsilon}\right) \log^3\left(\frac{1}{\delta}\right) \log^{3/2}\left(\frac{\log(1/\delta)}{\varepsilon}\right) \tag{2.5.1}$$

when $d = 2$ *and*

$$H_{[]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0,\delta), d_{\mathrm{H}}\bigr) \lesssim m\left\{\left(\frac{\delta}{\varepsilon}\right)^2 \log^6\left(\frac{1}{\delta}\right) + \left(\frac{\delta}{\varepsilon}\right)^{3/2} \log^7\left(\frac{1}{\delta}\right)\right\} \tag{2.5.2}$$

when $d = 3$.

See Propositions 2.6.8 and 2.6.9 for details of the initial stages of the proof, which deal with the case where f_0 is the uniform density $f_K := \mu_d(K)^{-1}\mathbb{1}_K$ on some polytope $K \in \mathcal{P}^m$. Here, we turn our attention to the general non-uniform case, where the support of f_0 may be unbounded. Writing $\mathcal{F}^1$ for the subclass of all log-1-affine densities in $\mathcal{F}_d$, we note that any $f \in \mathcal{F}^1$ must take the form $x \mapsto f_{K,\alpha}(x) := c_{K,\alpha}^{-1}\exp(-\alpha^\top x)\mathbb{1}_{\{x\in K\}}$, where $K \subseteq \mathbb{R}^d$ and $\alpha \in \mathbb{R}^d$ are the support and negative log-gradient of f respectively, and $c_{K,\alpha} := \int_K \exp(-\alpha^\top x)\,dx \in (0,\infty)$; see (2.7.4). It follows from the characterisation of $\mathcal{F}^1$ given in Proposition 2.7.4 that K and α satisfy the conditions of Proposition 2.7.2(ii), which in turn implies that $m_{K,\alpha} := \inf_{x\in K}\alpha^\top x$ is finite. In addition, let $M_{K,\alpha} := \sup_{x\in K}\alpha^\top x \in (-\infty,\infty]$, and for $t \in \mathbb{R}$, define the convex sets

$$\begin{aligned}
K_{\alpha,t} &:= K \cap \{x \in \mathbb{R}^d : \alpha^\top x = t\},\\
K^+_{\alpha,t} &:= K \cap \{x \in \mathbb{R}^d : \alpha^\top x \le t\},\\
\breve{K}_{\alpha,t} &:= K \cap \{x \in \mathbb{R}^d : t-1 \le \alpha^\top x \le t\},
\end{aligned}$$

which are all compact by Proposition 2.7.2; see Figure 2.2 for an illustration. Finally, we denote by $\mathcal{F}^1_\star$ the collection of all $f = f_{K,\alpha} \in \mathcal{F}^1$ for which $m_{K,\alpha} = 0$.

Proof of Proposition 2.5.1. For a fixed $d \in \{2,3\}$, let $\upsilon \equiv \upsilon_d := 2^{-3/2} \wedge \{d^{-1/2}(d+1)^{-(d-1)/2}\}$, $C \equiv C_d := 8d+7$ and $\varrho \equiv \varrho_d := \nu_d \wedge \upsilon_d\, e^{-C/2}\gamma(d,C)^{1/2}$, where $\gamma \equiv \gamma(d,C)$ and $\nu \equiv \nu_d$ are taken from Lemmas 2.7.6 and 2.7.15 respectively. For $0 < \varepsilon < \delta < \upsilon$, the important quantity $H_d(\delta,\varepsilon)$ is defined in Proposition 2.6.8.

Fix $0 < \varepsilon < \delta < \varrho$ and $m \in \mathbb{N}$ with $m \ge d$. It follows from Corollary 2.7.5 and the affine invariance of the Hellinger distance that we need only consider densities $f_0 = f_{K,\alpha} \in \mathcal{F}^1_\star \cap \mathcal{F}^1(\mathcal{P}^m)$, which have the property that $K \in \mathcal{P}^m$ and $m_{K,\alpha} = 0$. Since Proposition 2.6.9 handles the case $\alpha = 0$, we fix an arbitrary $f_{K,\alpha} \in \mathcal{F}^1_\star \cap \mathcal{F}^1(\mathcal{P}^m)$ with $\alpha \ne 0$, and set $L := \lceil M_{K,\alpha}\rceil \in \mathbb{N}\cup\{\infty\}$. Now define

$$K'_j := \begin{cases} K^+_{\alpha,C} & \text{for } j = C\\ \breve{K}_{\alpha,j} & \text{for each } j \in \mathbb{N} \text{ with } C+1 \le j \le L,\end{cases}$$

which is compact for all integers $C \le j \le L$. Note also that since $K \in \mathcal{P}^m$, it follows from Bruns and Gubeladze (2009, Theorem 1.6) that $K'_C \in \mathcal{P}^{m+1}$ and $K'_j \in \mathcal{P}^{m+2}$ for all integers $C+1 \le j \le L$.

Also, let a_+ be the smallest integer $C+1 \le j \le L$ such that $\delta^2 e^{j+1}\mu_d(\breve{K}_{\alpha,j})^{-1}c_{K,\alpha} \ge \upsilon^2$ if such a j exists, and let $a_+ = L+1$ otherwise. Since $(1/\tilde{\delta})^{d-1} \ge \log^{d-1}(1/\tilde{\delta}) \ge d(d+1)^{d-1}\upsilon^2\log^{d-1}(1/\tilde{\delta})$ for all $\tilde{\delta} \in (0,1)$, we deduce from (2.7.7) in Lemma 2.7.6 that

$$\frac{\delta^2 e^{t+1}c_{K,\alpha}}{\mu_d(\breve{K}_{\alpha,t})} \ge \frac{\delta^2 e^{t+1}c_{K,\alpha}}{dt^{d-1}\mu_d(K^+_{\alpha,1})} \ge \frac{\delta^2 e^t}{dt^{d-1}} \ge \upsilon^2$$

for all $t \ge (d+1)\log(1/\delta)$, and hence that $a_+ \lesssim \log(1/\delta)$. Next, set $u_j^2 := c\exp\{-(j-a_+)/2\}$ for each integer $a_+ \le j \le L$, where $c := 1 - e^{-1/2}$ is chosen to ensure that $\sum_{j=a_+}^L u_j^2 \le 1$, and also define

$$\varepsilon_j^2 := \begin{cases} 2\varepsilon^2/3 & \text{for } j = C \\ 2\varepsilon^2(a_+ - C)^{-1}/3 & \text{for } j = C+1,\ldots,a_+ - 1 \\ 2u_j^2\,\varepsilon^2/3 & \text{for } j = a_+,\ldots,L. \end{cases}$$

Since $K = \bigcup_{j=C}^{L} K'_j$ and $\sum_{j=C}^{L} \varepsilon_j^2 \leq 2\varepsilon^2$, we can write

$$H_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_{K,\alpha},\delta), d_{\mathrm{H}}\bigr) \leq H_{[\,]}\bigl(\varepsilon_C, \mathcal{G}(f_{K,\alpha},\delta), d_{\mathrm{H}}, K'_C\bigr) \tag{2.5.3}$$

$$+ \textstyle\sum_{j=C+1}^{a_+-1} H_{[\,]}\bigl(\varepsilon_j, \mathcal{G}(f_{K,\alpha},\delta), d_{\mathrm{H}}, K'_j\bigr) \tag{2.5.4}$$

$$+ \textstyle\sum_{j=a_+}^{L} H_{[\,]}\bigl(\varepsilon_j, \mathcal{G}(f_{K,\alpha},\delta), d_{\mathrm{H}}, K'_j\bigr), \tag{2.5.5}$$

and we now address each of the terms (2.5.3), (2.5.4) and (2.5.5) in turn. Note that while there are infinitely many summands in (2.5.5) when $M_{K,\alpha} = L = \infty$, it will follow from the bounds we obtain that only finitely many of these are non-zero.

For (2.5.3), let $A_C := c_{K,\alpha}/\mu_d(K'_C)$, which by Lemma 2.7.6 satisfies $e^{-C} \leq A_C \leq \gamma^{-1}$. For $f \in \mathcal{G}(f_{K,\alpha},\delta)$, define $\tilde{f}_C \colon \mathbb{R}^d \to [0,\infty)$ by $\tilde{f}_C(x) := A_C \exp(\alpha^\top x) f(x) \mathbb{1}_{\{x \in K'_C\}}$ and observe that

$$\delta^2 \geq \int_{K'_C} (f_C^{1/2} - f_{K,\alpha}^{1/2})^2 = \int_{K'_C} \frac{e^{-\alpha^\top x}}{A_C} \bigl\{\tilde{f}_C^{1/2}(x) - f_{K'_C}^{1/2}(x)\bigr\}^2 \, dx \geq \frac{e^{-C}}{A_C} \int_{K'_C} (\tilde{f}_C^{1/2} - f_{K'_C}^{1/2})^2,$$

which shows that $\tilde{f}_C \in \mathcal{G}\bigl(f_{K'_C}, A_C^{1/2} e^{C/2}\delta\bigr)$. Since $\delta < \varrho < \upsilon e^{-C/2}\gamma^{1/2}$, it follows from the above bounds on A_C that

$$\delta \leq A_C^{1/2} e^{C/2}\delta < \upsilon < 2^{-3/2} \quad \text{and} \quad A_C^{-1/2}\varepsilon_C^{-1} \lesssim \varepsilon^{-1}. \tag{2.5.6}$$

Recalling that $K'_C \in \mathcal{P}^{m+1}$, we can now apply Proposition 2.6.9 to deduce that there exists an $\bigl(A_C^{1/2}\varepsilon_C\bigr)$-Hellinger bracketing set $\{[\tilde{g}_\ell^L, \tilde{g}_\ell^U] : 1 \leq \ell \leq N_C\}$ for $\mathcal{G}\bigl(f_{K'_C}, A_C^{1/2} e^{C/2}\delta\bigr)$ such that

$$\log N_C \lesssim (m+1) H_d\bigl(A_C^{1/2} e^{C/2}\delta, A_C^{1/2}\varepsilon_C\bigr) \lesssim m H_d(\delta, \varepsilon). \tag{2.5.7}$$

We see that $\{f\mathbb{1}_{K'_C} : f \in \mathcal{G}(f_{K,\alpha},\delta)\}$ is covered by the brackets $\{[g_\ell^L, g_\ell^U] : 1 \leq \ell \leq N_C\}$ defined by

$$g_\ell^L(x) := A_C^{-1} \exp(-\alpha^\top x)\, \tilde{g}_\ell^L(x); \quad g_\ell^U(x) := A_C^{-1} \exp(-\alpha^\top x)\, \tilde{g}_\ell^U(x).$$

Moreover, $\exp(-\alpha^\top x) \leq 1$ for all $x \in K'_C$, so

$$\int_{K'_C} \Bigl(\sqrt{g_\ell^U} - \sqrt{g_\ell^L}\Bigr)^2 = A_C^{-1} \int_{K'_C} \Bigl(\sqrt{\tilde{g}_\ell^U(x)} - \sqrt{\tilde{g}_\ell^L(x)}\Bigr)^2 \exp(-\alpha^\top x)\, dx \leq \varepsilon_C^2$$

for all $1 \leq \ell \leq N_C$. Together with (2.5.7), this implies that

$$H_{[\,]}\bigl(\varepsilon_C, \mathcal{G}(f_{K,\alpha},\delta), d_{\mathrm{H}}, K'_C\bigr) \leq \log N_C \lesssim m H_d(\delta, \varepsilon). \tag{2.5.8}$$

For (2.5.4), fix an integer $C+1 \leq j \leq a_+ - 1$ (if such a j exists) and let $A_j := c_{K,\alpha}/\mu_d(K'_j)$. For $f \in \mathcal{G}(f_{K,\alpha},\delta)$, define $\tilde{f}_j \colon \mathbb{R}^d \to [0,\infty)$ by $\tilde{f}_j(x) := A_j \exp(\alpha^\top x) f(x) \mathbb{1}_{\{x \in K'_j\}}$. Now

$$\delta^2 \geq \int_{K'_j} (f^{1/2} - f_{K,\alpha}^{1/2})^2 = \int_{K'_j} \frac{e^{-\alpha^\top x}}{A_j} \bigl\{\tilde{f}_j^{1/2}(x) - f_{K'_j}^{1/2}(x)\bigr\}^2 \, dx \geq \frac{e^{-j}}{A_j} \int_{K'_j} (\tilde{f}_j^{1/2} - f_{K'_j}^{1/2})^2,$$

so $\tilde{f}_j \in \mathcal{G}\big(f_{K'_j}, A_j^{1/2}\, e^{j/2}\, \delta\big)$. Since $j \leq a_+ - 1$, it follows from the definition of a_+ that $A_j < \delta^{-2} \upsilon^2\, e^{-(j+1)}$. In addition, since $K'_j \subseteq K^+_{\alpha,j}$, we can apply Lemma 2.7.6 to deduce that $A_j \geq c_{K,\alpha}/\mu_d(K^+_{\alpha,j}) \geq e^{-j}$. Therefore,

$$\delta \leq A_j^{1/2}\, e^{j/2}\, \delta < \upsilon < 2^{-3/2} \quad \text{and} \quad A_j^{-1/2}\, e^{-(j-1)/2} \lesssim 1.$$

Since $K'_j \in \mathcal{P}^{m+2}$, we can apply Proposition 2.6.9 to deduce that there exists an $(A_j^{1/2}\, e^{(j-1)/2}\, \varepsilon_j)$-Hellinger bracketing set $\{[\tilde{g}^L_\ell, \tilde{g}^U_\ell] : 1 \leq \ell \leq N_j\}$ for $\mathcal{G}\big(f_{K'_j}, A_j^{1/2}\, e^{j/2}\, \delta\big)$ such that

$$\log N_j \lesssim (m+2) H_d\big(A_j^{1/2}\, e^{j/2}\, \delta, A_j^{1/2}\, e^{(j-1)/2}\, \varepsilon_j\big) \lesssim m H_d(\delta, \varepsilon_j). \tag{2.5.9}$$

We see that $\{f \mathbb{1}_{K'_j} : f \in \mathcal{G}(f_{K,\alpha}, \delta)\}$ is covered by the brackets $\{[g^L_\ell, g^U_\ell] : 1 \leq \ell \leq N_j\}$ defined by

$$g^L_\ell(x) := A_j^{-1} \exp(-\alpha^\top x)\, \tilde{g}^L_\ell(x); \quad g^U_\ell(x) := A_j^{-1} \exp(-\alpha^\top x)\, \tilde{g}^U_\ell(x).$$

Moreover, $\exp(-\alpha^\top x) \leq e^{-(j-1)}$ for all $x \in K'_j$, so

$$\int_{K'_j} \Big(\sqrt{g^U_\ell} - \sqrt{g^L_\ell}\Big)^2 = A_j^{-1} \int_{K'_j} \Big(\sqrt{\tilde{g}^U_\ell(x)} - \sqrt{\tilde{g}^L_\ell(x)}\Big)^2 \exp(-\alpha^\top x)\, dx \leq \varepsilon_j^2$$

for all $1 \leq \ell \leq N_j$. Together with (2.5.9) and the fact that $a_+ \lesssim \log(1/\delta)$, this implies that

$$\sum_{j=C+1}^{a_+-1} H_{[\,]}\big(\varepsilon_j, \mathcal{G}(f_{K,\alpha}, \delta), d_{\mathrm{H}}, K'_j\big) \lesssim \log(1/\delta)\, m H_d\big(\delta,\, \varepsilon/\log(1/\delta)^{1/2}\big),$$

which is bounded above up to a universal constant by

$$m \left(\frac{\delta}{\varepsilon}\right) \log^3\left(\frac{1}{\delta}\right) \log^{3/2}\left(\frac{\log(1/\delta)}{\varepsilon}\right) \tag{2.5.10}$$

when $d = 2$ and

$$m \left\{ \left(\frac{\delta}{\varepsilon}\right)^2 \log^6\left(\frac{1}{\delta}\right) + \left(\frac{\delta}{\varepsilon}\right)^{3/2} \log^7\left(\frac{1}{\delta}\right) \right\} \tag{2.5.11}$$

when $d = 3$.

For (2.5.5), if $L \geq C + 1$, consider $f = e^\phi \in \mathcal{G}(f_{K,\alpha}, \delta)$ and define $\psi \equiv \tilde{\phi}_{K,\alpha} \colon \mathbb{R}^d \to [-\infty, \infty)$ by $\psi(x) := \phi(x) + \alpha^\top x + \log c_{K,\alpha}$, as in the statement of Lemma 2.7.15. First, we claim that

$$\psi(x) \leq \frac{4d+2}{a_+ - 2}\, \alpha^\top x \tag{2.5.12}$$

for all $x \in K \setminus K^+_{\alpha,\, a_+-1}$. To see this, first set $\tilde{K} := K^+_{\alpha,\, a_+-1}$ and $\tilde{A} := c_{K,\alpha}/\mu_d(\tilde{K})$, and define $\tilde{f} \colon \mathbb{R}^d \to [0, \infty)$ by $\tilde{f}(x) := \tilde{A} \exp(\alpha^\top x) f(x) \mathbb{1}_{\{x \in \tilde{K}\}}$. Observe that

$$\log \tilde{f}(x) = \log f(x) + \alpha^\top x + \log c_{K,\alpha} - \log \mu_d(\tilde{K}) = \psi(x) - \log \mu_d(\tilde{K}).$$

By similar arguments to those given above, we deduce that $\tilde{f} \in \mathcal{G}\big(f_{\tilde{K}}, \tilde{A}^{1/2}\, e^{(a_+-1)/2}\, \delta\big)$. Moreover, if $a_+ \geq C + 2$, then it follows from the definitions of a_+ and υ that

$$\tilde{A} e^{a_+-1} \delta^2 \leq \mu_d(\check{K}_{\alpha,\, a_+-1})^{-1} c_{K,\alpha}\, e^{a_+-1} \delta^2 < e^{-1} \upsilon^2 < 2^{-3}.$$

Otherwise, if $a_+ = C+1$, then recall from (2.5.6) that

$$\tilde{A}e^{a_+-1}\delta^2 = A_C\, e^C\delta^2 < \upsilon^2 < 2^{-3}.$$

Therefore, in all cases, Lemma 2.7.14(ii) implies that $\log \tilde{f}(x) \leq 2^{7/2}d\,(\tilde{A}^{1/2}\,e^{(a_+-1)/2}\,\delta) - \log\mu_d(\tilde{K})$ for all $x \in \tilde{K}$, and hence that $\psi \leq 4d$ on $K_{\alpha,\,a_+-1}$. On the other hand, we know from Lemma 2.7.15 that there exists some $x_- \in K^+_{\alpha,1}$ such that $\psi(x_-) > -2$. Now if $x \in K$ and $\alpha^\top x > a_+ - 1$, then $s := (a_+ - 1 - \alpha^\top x_-)/(\alpha^\top x - \alpha^\top x_-)$ satisfies $1 \geq s \geq (a_+-2)/(\alpha^\top x - 1) > 0$, and $w := sx + (1-s)x_-$ lies in $K_{\alpha,\,a_+-1}$. It then follows from the concavity of ψ that

$$\psi(x) \leq \frac{1}{s}\,\psi(w) - \frac{1-s}{s}\,\psi(x_-) \leq \frac{4d}{s} + \frac{2\,(1-s)}{s} = \frac{4d+2}{s} - 2 < \frac{4d+2}{a_+-2}\,\alpha^\top x,$$

which yields (2.5.12), as required.

Now fix an integer $a_+ \leq j \leq L$ (if such a j exists). First, recalling the definition of a_+, we deduce from the bound (2.7.7) in Lemma 2.7.6 that

$$\frac{\mu_d(K_j')}{c_{K,\alpha}\,e^{a_+}} \leq \left(\frac{j}{a_+-1}\right)^{d-1}\frac{\mu_d(\breve{K}_{\alpha,\,a_+})}{c_{K,\alpha}\,e^{a_+}} \leq e\upsilon^{-2}\delta^2\left(\frac{j}{a_+-1}\right)^{d-1}. \tag{2.5.13}$$

Also, it follows from (2.5.12) that if $f \in \mathcal{G}(f_{K,\alpha},\delta)$, then the function $\tilde{f}_j\colon \mathbb{R}^d \to [0,\infty)$ defined by $\tilde{f}_j(x) := c_{K,\alpha}\exp(\alpha^\top x)f(x)\mathbb{1}_{\{x\in K_j'\}}$ belongs to $\mathcal{G}_{-\infty,B_j}(K_j') := \bigl\{g\mathbb{1}_{K_j'} : g \in \mathcal{G},\, g\mathbb{1}_{K_j'} \leq e^{B_j}\bigr\}$, where $B_j := (4d+2)j/(a_+-2)$. Now if $\{[\tilde{g}_\ell^L, \tilde{g}_\ell^U] : 1 \leq \ell \leq N\}$ is a $(c_{K,\alpha}^{1/2}e^{(j-1)/2}\,\varepsilon_j)$-Hellinger bracketing set for $\mathcal{G}_{-\infty,B_j}(K_j')$, then $\{f\mathbb{1}_{K_j'} : f \in \mathcal{G}(f_{K,\alpha},\delta)\}$ is covered by the brackets $\{[g_\ell^L, g_\ell^U] : 1 \leq \ell \leq N\}$ defined by

$$g_\ell^L(x) := c_{K,\alpha}^{-1}\exp(-\alpha^\top x)\,\tilde{g}_\ell^L(x); \quad g_\ell^U(x) := c_{K,\alpha}^{-1}\exp(-\alpha^\top x)\,\tilde{g}_\ell^U(x).$$

Moreover, $\exp(-\alpha^\top x) \leq e^{-(j-1)}$ for all $x \in K_j'$, so

$$\int_{K_j'}\left(\sqrt{g_\ell^U} - \sqrt{g_\ell^L}\right)^2 = c_{K,\alpha}^{-1}\int_{K_j'}\left(\sqrt{\tilde{g}_\ell^U(x)} - \sqrt{\tilde{g}_\ell^L(x)}\right)^2\exp(-\alpha^\top x)\,dx \leq \varepsilon_j^2$$

for all $1 \leq \ell \leq N$. Recalling that $a_+ \geq C = 8d+7$ and that h_d is a decreasing function for $d = 2,3$, we now apply (2.5.13) and the bound (2.6.35) from Proposition 2.6.7 to deduce that

$$\begin{aligned}
H_{[\,]}\bigl(\varepsilon_j, \mathcal{G}(f_{K,\alpha},\delta), d_{\mathrm{H}}, K_j'\bigr) &\leq H_{[\,]}\bigl(c_{K,\alpha}^{1/2}e^{(j-1)/2}\,\varepsilon_j, \mathcal{G}_{-\infty,B_j}(K_j'), d_{\mathrm{H}}\bigr)\\
&\lesssim h_d\left(\frac{c_{K,\alpha}^{1/2}e^{(j-1)/2}\,\varepsilon_j}{\mu_d(K_j')^{1/2}\exp\left\{\frac{(4d+2)\,j}{2(a_+-2)}\right\}}\right)\\
&\lesssim h_d\left(\left\{\frac{c_{K,\alpha}}{\mu_d(K_j')}\right\}^{1/2}\frac{e^{(j-a_+)/2}e^{a_+/2}e^{-(j-a_+)/4}\,\varepsilon}{\exp\left\{\frac{(4d+2)(j-a_+)}{2(a_+-2)} + \frac{(4d+2)\,a_+}{2(a_+-2)}\right\}}\right)\\
&\lesssim h_d\left(\left\{\frac{c_{K,\alpha}\,e^{a_+}}{\mu_d(K_j')}\right\}^{1/2}\varepsilon\exp\left\{-\left(\frac{4d+2}{2(a_+-2)} - \frac{1}{4}\right)(j-a_+)\right\}\right)\\
&\lesssim h_d\left(\frac{\varepsilon}{\delta}\left(\frac{a_+-1}{j}\right)^{\frac{d-1}{2}}\exp\left\{-\left(\frac{4d+2}{2(a_+-2)} - \frac{1}{4}\right)(j-a_+)\right\}\right)\\
&\lesssim h_d\left(\frac{\varepsilon}{\delta}\left(\frac{a_+-1}{j}\right)^{\frac{d-1}{2}}\exp\left\{-\left(\frac{4d+2}{2(8d+5)} - \frac{1}{4}\right)(j-a_+)\right\}\right),
\end{aligned}$$

and we note that $\frac{4d+2}{2(8d+5)} - \frac{1}{4} < 0$. Thus, when $d = 2$, the final expression above is bounded above by a constant multiple of

$$\frac{\delta}{\varepsilon} \log^{3/2}\left(\frac{\delta}{\varepsilon}\right) j^{1/2} (\log^{3/2} j) \exp\left\{-\left(\frac{1}{4} - \frac{4d+2}{2(8d+5)}\right)(j - a_+)\right\},$$

where we have used the fact that $\log_+(ax) \leq (1 + \log a)\log_+ x$ for all $x > 0$ and $a \geq 1$. It follows that

$$\sum_{j=a_+}^{L} H_{[]}\bigl(\varepsilon_j, \mathcal{G}(f_{K,\alpha}, \delta), d_{\mathrm{H}}, K_j'\bigr) \lesssim \frac{\delta}{\varepsilon} \log^{3/2}\left(\frac{\delta}{\varepsilon}\right) \tag{2.5.14}$$

when $d = 2$. Similarly, when $d = 3$, we conclude that

$$\sum_{j=a_+}^{L} H_{[]}\bigl(\varepsilon_j, \mathcal{G}(f_{K,\alpha}, \delta), d_{\mathrm{H}}, K_j'\bigr) \lesssim \left(\frac{\delta}{\varepsilon}\right)^2. \tag{2.5.15}$$

Combining (2.5.3), (2.5.4), (2.5.5), (2.5.8), (2.5.10), (2.5.11), (2.5.14) and (2.5.15) yields the result. □

We are now in a position to give the proof of Theorem 2.2.3.

Proof of Theorem 2.2.3. By the affine equivariance of the log-concave maximum likelihood estimator (Dümbgen et al., 2011, Remark 2.4) and the affine invariance of d_{H}, we may assume without loss of generality that $f_0 \in \mathcal{F}_d^{0,I}$. In addition, by Kim and Samworth (2016, Lemma 6), we have

$$\sup_{f_0 \in \mathcal{F}_d^{0,I}} \mathbb{P}(\hat{f}_n \notin \tilde{\mathcal{F}}_d^{1,\eta_d}) = O(n^{-1}), \tag{2.5.16}$$

where $\tilde{\mathcal{F}}_d^{1,\eta_d}$ is the class of 'near-isotropic' log-concave densities defined at the start of Section 2.5.1. For fixed $f_0 \in \mathcal{F}_d$ and $m \geq d$, let

$$\Delta := \inf_{\substack{f \in \mathcal{F}^1(\mathcal{P}^m) \\ \mathrm{supp}\, f_0 \subseteq \mathrm{supp}\, f}} d_{\mathrm{H}}^2(f_0, f).$$

First we consider the case $d = 2$ and assume for the time being that $\Delta \leq \varrho_2/2$, where ϱ_2 is taken from Proposition 2.5.1. If $\delta \in (0, \varrho_2 - \Delta)$, then for all $\eta' \in (0, \varrho_2 - \Delta - \delta)$, there exists $f \in \mathcal{F}^1(\mathcal{P}^m)$ with $\mathrm{supp}\, f_0 \subseteq \mathrm{supp}\, f$ such that $d_{\mathrm{H}}(f_0, f) \leq \Delta + \eta'$. It follows from the triangle inequality that $\mathcal{F}(f_0, \delta) \subseteq \mathcal{F}(f, \delta + \Delta + \eta') \subseteq \mathcal{F}(f, \varrho_2)$, and we deduce from the first bound (2.5.1) in Proposition 2.5.1 that

$$H_{[]}\bigl(2^{1/2}\varepsilon, \mathcal{F}(f_0, \delta), d_{\mathrm{H}}\bigr) \lesssim m\left(\frac{\delta + \Delta + \eta'}{\varepsilon}\right) \log^3\left(\frac{1}{\delta}\right) \log^{3/2}\left(\frac{\log(1/\delta)}{\varepsilon}\right).$$

But since $\eta' \in (0, \varrho_2 - \Delta - \delta)$ was arbitrary, it follows that

$$H_{[]}\bigl(2^{1/2}\varepsilon, \mathcal{F}(f_0, \delta), d_{\mathrm{H}}\bigr) \lesssim m\left(\frac{\delta + \Delta}{\varepsilon}\right) \log^3\left(\frac{1}{\delta}\right) \log^{3/2}\left(\frac{\log(1/\delta)}{\varepsilon}\right) \tag{2.5.17}$$

and hence that

$$\int_{\delta^2/2^{13}}^{\delta} H_{[]}^{1/2}\bigl(\varepsilon, \mathcal{F}(f_0, \delta), d_{\mathrm{H}}\bigr)\, d\varepsilon \lesssim m^{1/2}(\delta + \Delta)^{1/2} \log^{3/2}\left(\frac{1}{\delta}\right) \int_0^{\delta} \varepsilon^{-1/2} \log^{3/4}\left(\frac{\log(1/\delta)}{\varepsilon}\right) d\varepsilon. \tag{2.5.18}$$

Now for any $a > e\delta$, we can integrate by parts to establish that

$$\int_0^\delta \varepsilon^{-1/2} \log^{3/4}\Bigl(\frac{a}{\varepsilon}\Bigr)\, d\varepsilon = a^{1/2}\int_{\log(a/\delta)}^\infty u^{3/4}e^{-u/2}\,du = 2\delta^{1/2}\log^{3/4}\Bigl(\frac{a}{\delta}\Bigr) + \frac{3a^{1/2}}{2}\int_{\log(a/\delta)}^\infty \frac{e^{-u/2}}{u^{1/4}}\,du$$
$$\leq 5\delta^{1/2}\log^{3/4}(a/\delta). \tag{2.5.19}$$

Thus, setting $a := \log(1/\delta)$ and combining the bounds in (2.5.18) and (2.5.19), we see that

$$\frac{1}{\delta^2}\int_{\delta^2/2^{13}}^\delta H_{[]}^{1/2}\bigl(\varepsilon, \mathcal{F}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta_2}, d_{\mathrm{H}}\bigr)\,d\varepsilon \lesssim m^{1/2}\Bigl(\frac{\delta+\Delta}{\delta^3}\Bigr)^{1/2}\log^{9/4}\Bigl(\frac{1}{\delta}\Bigr),$$

where the right hand side is a decreasing function of $\delta \in (0, \varrho_2 - \Delta)$. On the other hand, if $\delta \geq \varrho_2 - \Delta$, which is at least $\varrho_2/2$, then it follows from Kim and Samworth (2016, Theorem 4) that

$$H_{[]}(\varepsilon, \tilde{\mathcal{F}}^{1,\eta_2}, d_{\mathrm{H}}) \lesssim h_2(\varepsilon) \lesssim \frac{1}{\varepsilon}\log_+^{3/2}\Bigl(\frac{1}{\varepsilon}\Bigr) \lesssim \frac{\delta}{\varepsilon}\log_+^{3/2}\Bigl(\frac{1}{\varepsilon}\Bigr)$$

and hence that

$$\frac{1}{\delta^2}\int_{\delta^2/2^{13}}^\delta H_{[]}^{1/2}\bigl(\varepsilon, \mathcal{F}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta_2}, d_{\mathrm{H}}\bigr)\,d\varepsilon \lesssim \frac{1}{\delta}\log_+^{3/4}\Bigl(\frac{1}{\delta}\Bigr).$$

Consequently, there exists a universal constant $C_2' > 0$ such that the function $\Psi_2\colon (0,\infty)\to(0,\infty)$ defined by

$$\Psi_2(\delta) := C_2'\, m^{1/2}\,\delta^{1/2}(\delta+\Delta)^{1/2}\,\log_+^{9/4}(1/\delta)$$

satisfies $\Psi_2(\delta) \geq \delta \vee \int_{\delta^2/2^{13}}^\delta H_{[]}^{1/2}(\varepsilon, \mathcal{F}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta_2}, d_{\mathrm{H}})\,d\varepsilon$ for all $\delta > 0$ and has the property that $\delta \mapsto \delta^{-2}\,\Psi_2(\delta)$ is decreasing. Setting $c_2 := 2^{69/4}\,C_2' \vee 1$ and $\delta_n := (c_2^2\, mn^{-1}\log^{9/2} n + \Delta^2)^{1/2}$, we have $\Delta \leq \delta_n$ and $\delta_n^{-1} \leq c_2^{-1}m^{-1/2}\,n^{1/2}\log^{-9/4} n \leq n^{1/2}$, so

$$\delta_n^{-2}\,\Psi_2(\delta_n) \leq 2^{1/2}\,C_2'\,m^{1/2}\,\delta_n^{-1}\log^{9/4}(n^{1/2}) \leq 2^{-19}n^{1/2}. \tag{2.5.20}$$

We are now in a position to apply van de Geer (2000, Corollary 7.5), which is restated as Theorem 10 in the online supplement to Kim et al. (2018). It follows from this, (2.5.16) and the bound (2.6.2) from Lemma 2.6.1 that there are universal constants $\bar{C}, c, c', c'' > 0$ such that

$$\begin{aligned}
\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} &\leq \int_0^{8d\log n} \mathbb{P}\bigl[\{d_X^2(\hat{f}_n, f_0) \geq t\}\cap\{\hat{f}_n \in \tilde{\mathcal{F}}^{1,\eta_2}\}\bigr]\,dt \\
&\qquad + (8d\log n)\,\mathbb{P}(\hat{f}_n \notin \tilde{\mathcal{F}}^{1,\eta_2}) + \int_{8d\log n}^\infty \mathbb{P}\{d_X^2(\hat{f}_n, f_0) \geq t\}\,dt \\
&\leq \delta_n^2 + \int_{\delta_n^2}^\infty c\exp(-nt/c^2)\,dt + c'n^{-1}\log n + c''n^{-3} \leq \delta_n^2 + 2c'n^{-1}\log n \\
&\leq \frac{\bar{C}m}{n}\log^{9/2} n + \Delta^2
\end{aligned} \tag{2.5.21}$$

for all $n \geq 3$, provided that $\Delta \leq \varrho_2/2$. On the other hand, when $\Delta > \varrho_2/2$, observe that by Theorem 2.6.2, which is a small modification of Kim and Samworth (2016, Theorem 5), we have $\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \lesssim n^{-2/3}\log n \lesssim (\varrho_2/2)^2 \leq \Delta^2$. We have now established the $d = 2$ case of the desired result.

The proof for the case $d = 3$ is very similar in most respects, except that the first term in the local bracketing entropy bound (2.5.2) from Proposition 2.5.1 gives rise to a divergent entropy integral. If

$\Delta \leq \varrho_3/2$, then

$$\frac{1}{\delta^2}\int_{\delta^2/2^{13}}^{\delta} H_{[]}^{1/2}(\varepsilon, \mathcal{F}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta_3}, d_{\mathrm{H}})\,d\varepsilon \lesssim m\left(\frac{\delta+\Delta}{\delta^2}\right)\log_+^4\left(\frac{1}{\delta}\right)$$

for all $\delta > 0$, where we once again appeal to the global entropy bound

$$H_{[]}(\varepsilon, \tilde{\mathcal{F}}^{1,\eta_3}, d_{\mathrm{H}}) \lesssim h_3(\varepsilon) \lesssim \frac{1}{\varepsilon^2}$$

from Kim and Samworth (2016, Theorem 4) to handle the case $\delta \geq \varrho_3 - \Delta$. We conclude as above that there exists $C_3' > 0$ such that the function $\Psi_3\colon (0,\infty)\to(0,\infty)$ defined by

$$\Psi_3(\delta) := C_3'\, m^{1/2}(\delta+\Delta)\log_+^4(1/\delta)$$

has all the required properties. Also, if we set $c_3 := 2^{16}\, C_3' \vee 1$, then $\delta_n := \bigl(c_3^2\, mn^{-1}\log^8 n + \Delta^2\bigr)^{1/2}$ satisfies $\delta_n^{-2}\,\Psi_3(\delta_n) \leq 2^{-19}n^{1/2}$ for all $n \geq 4$. The rest of the argument above then goes through, and we once again use the worst-case bound $\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \lesssim n^{-1/2}\log n$ from Theorem 2.6.2 to handle the case where $\Delta > \varrho_3/2$. □

Proof of Proposition 2.2.4. Observe that in Proposition 2.6.9, the polylogarithmic exponents in the local bracketing entropy bounds for uniform densities on polytopes in $\mathcal{P}^m$ are smaller than those that appear in Proposition 2.5.1. We can therefore exploit this and deduce Proposition 2.2.4 from Proposition 2.6.9 in the same way as Theorem 2.2.3 is derived from Proposition 2.5.1. We omit the details for brevity. □

Now that we have established our main novel results of this section, the proof of Theorem 2.2.2 is broadly similar to that of the univariate oracle inequality stated as Theorem 3 in Kim et al. (2018), so our exposition will be brief, and we will seek to emphasise the main points of difference.

Proof of Theorem 2.2.2. Fix $f_0 \in \mathcal{F}$ and an arbitrary $f \in \bigcup_{m\in\mathbb{N}}\mathcal{F}^k(\mathcal{P}^m)$ such that $\mathrm{KL}(f_0, f) < \infty$. Note that we must have $\operatorname{supp} f_0 \subseteq \operatorname{supp} f$. Proposition 2.2.1 yields a polyhedral subdivision $E_1,\dots,E_\ell$ of $\operatorname{supp} f \in \mathcal{P}$ with $\ell := \kappa(f) \leq k$ such that $\log f$ is affine on each E_j, and recall that $\Gamma(f) = \sum_{j=1}^{\ell} d_j$, where $d_j := |\mathfrak{F}(E_j)|$. Setting $p_j := \int_{E_j} f_0$ and $q_j := \int_{E_j} f$ for each $j \in \{1,\dots,\ell\}$, we see that $\sum_{j=1}^{\ell} p_j = \sum_{j=1}^{\ell} q_j = 1$. Moreover, let $N_j := \sum_{i=1}^{n}\mathbb{1}_{\{X_i\in E_j\}}$ for each $j \in \{1,\dots,\ell\}$, and partition the set of indices $\{1,\dots,\ell\}$ into the subsets $J_1 := \{j : N_j \geq d+1\}$ and $J_2 := \{j : N_j \leq d\}$. Then $|J_2| \leq d\ell$ and

$$d_X^2(\hat{f}_n, f_0) \leq \frac{1}{n}\sum_{j\in J_1}\sum_{i:X_i\in E_j}\log\frac{\hat{f}_n(X_i)}{f_0(X_i)} + \frac{d\ell}{n}\max_{1\leq i\leq n}\log\frac{\hat{f}_n(X_i)}{f_0(X_i)}. \tag{2.5.22}$$

The bound (2.6.1) from Lemma 2.6.1 controls the expectation of the second term on the right hand side of (2.5.22), so it remains to handle the first term. For each $j \in J_1$, let $f_0^{(j)}, f^{(j)} \in \mathcal{F}$ be the functions defined by $f_0^{(j)}(x) := p_j^{-1}f_0(x)\mathbb{1}_{\{x\in E_j\}}$ and $f^{(j)}(x) := q_j^{-1}f(x)\mathbb{1}_{\{x\in E_j\}}$. We also denote by $\hat{f}^{(j)}$ the maximum likelihood estimator based on $\{X_1,\dots,X_n\}\cap E_j$, which exists and is unique with probability 1 for each $j \in J_1$ (Dümbgen et al., 2011, Theorem 2.2). Writing $M_1 := \sum_{j\in J_1} N_j$ and arguing as in Kim et al. (2018), we find that

$$\sum_{j\in J_1}\sum_{i:X_i\in E_j}\log\hat{f}_n(X_i) \leq \sum_{j\in J_1}\sum_{i:X_i\in E_j}\log\frac{N_j\hat{f}^{(j)}(X_i)}{M_1}.$$

It follows that

$$
\begin{aligned}
\frac{1}{n}\mathbb{E}\Biggl(\sum_{j\in J_1}\sum_{i:X_i\in E_j}\log\frac{\hat{f}_n(X_i)}{f_0(X_i)}\Biggr) &\leq \frac{1}{n}\mathbb{E}\Biggl(\sum_{j\in J_1}\sum_{i:X_i\in E_j}\log\frac{N_j\hat{f}^{(j)}(X_i)/M_1}{p_jf_0^{(j)}(X_i)}\Biggr)\\
&= \frac{1}{n}\mathbb{E}\Biggl(\sum_{j\in J_1}\sum_{i:X_i\in E_j}\log\frac{\hat{f}^{(j)}(X_i)}{f_0^{(j)}(X_i)}\Biggr)+\mathbb{E}\Biggl(\sum_{j\in J_1}\frac{N_j}{n}\log\frac{N_j}{np_j}\Biggr)+\mathbb{E}\biggl(\frac{M_1}{n}\log\frac{n}{M_1}\biggr) \qquad (2.5.23)\\
&=: r_1+r_2+r_3.
\end{aligned}
$$

To bound r_1, we observe that $f^{(j)}\in\mathcal{F}^1(\mathcal{P}^{d_j})$ and $\mathrm{supp}\, f_0^{(j)}\subseteq\mathrm{supp}\, f^{(j)}$ for each $j\in J_1$. Consequently, after conditioning on the set of random variables $\{N_j : j=1,\ldots,\ell\}$, we can apply the risk bound in Theorem 2.2.3 to each $f_0^{(j)}$ and the corresponding $\hat{f}^{(j)}$ to deduce that

$$
\begin{aligned}
r_1 &\leq \frac{1}{n}\mathbb{E}\Biggl(\sum_{j\in J_1}N_j\Biggl\{\frac{\bar{C}d_j}{N_j}\log^{\gamma_d}N_j+\inf_{\substack{f_1\in\mathcal{F}^1(\mathcal{P}^{d_j})\\ \mathrm{supp}\, f_0^{(j)}\subseteq\mathrm{supp}\, f_1}} d_{\mathrm{H}}^2(f_0^{(j)},f_1)\Biggr\}\Biggr)\\
&\leq \frac{\bar{C}\,\Gamma(f)}{n}\log^{\gamma_d}n+\sum_{j=1}^{\ell}p_j\,d_{\mathrm{H}}^2(f_0^{(j)},f^{(j)})\\
&\leq \frac{\bar{C}\,\Gamma(f)}{n}\log^{\gamma_d}n+\mathrm{KL}(f_0,f), \qquad (2.5.24)
\end{aligned}
$$

where the penultimate inequality follows as in the proof of Kim et al. (2018, Theorem 3). Moreover,

$$
r_2\leq\sum_{j=1}^{\ell}\mathbb{E}\biggl\{\frac{N_j}{n}\biggl(\frac{N_j}{np_j}-1\biggr)\biggr\}-\mathbb{E}\Biggl(\sum_{j\in J_2}\frac{N_j}{n}\log\frac{N_j}{np_j}\Biggr)\leq\frac{\ell}{n}+\frac{d\ell}{n}\log n. \qquad (2.5.25)
$$

Finally, for r_3, we first suppose that $d\ell<n/2$, in which case $M_1/n\geq 1-(d\ell)/n>1/2$. Thus, arguing as in Kim et al. (2018), we deduce that $r_3\leq(2\ell d)/n$. Together with (2.5.23), (2.5.24), (2.5.25) and the fact that $\ell\leq\Gamma(f)$, this implies that the desired bound (2.2.2) holds whenever $d\ell<n/2$. On the other hand, if $d\ell\geq n/2$, then $\Gamma(f)/n\gtrsim 1$ and we can apply Lemma 2.6.1 again to conclude that

$$
\mathbb{E}\{d_X^2(\hat{f}_n,f_0)\}\leq\mathbb{E}\biggl(\max_{1\leq i\leq n}\log\frac{\hat{f}_n(X_i)}{f_0(X_i)}\biggr)\lesssim\log n\lesssim\frac{\Gamma(f)}{n}\log^{\gamma_d}n.
$$

This completes the proof of (2.2.2). The final assertion of Theorem 2.2.2 follows from Lemma 2.7.12 in the case $d=2$ and from the final assertion of Proposition 2.2.1 in the case $d=3$. □

2.5.2 Proofs of results in Section 2.3

Proof of Theorem 2.3.1. As in the proof of Theorem 2.2.3, we apply some empirical process theory to convert the local bracketing entropy bound in Proposition 2.6.11 into a statistical risk bound. Fix $f_0\in\mathcal{F}_3$, $m\geq d+1=4$ and $\theta\in(1,\infty)$, and let

$$
\Delta := \inf_{\substack{f\in\mathcal{F}^{[\theta]}(\mathcal{P}^m)\\ \mathrm{supp}\, f_0\subseteq\mathrm{supp}\, f}} d_{\mathrm{H}}^2(f_0,f).
$$

Suppose first that $\Delta<(8\theta)^{-1/2}/2=:\theta'/2$. If $\delta\in(0,\theta'-\Delta)$, then by analogy with the derivation of (2.5.17) in the proof of Theorem 2.2.3, we deduce from Proposition 2.6.11 and the triangle inequality that

$$\begin{aligned}&H_{[\,]}\big(2^{1/2}\varepsilon, \mathcal{F}(f_0,\delta), d_{\mathrm{H}}\big)\\&\quad\lesssim m\biggl\{\frac{\log^{3/2}\theta + (\delta+\Delta)^{3/5}}{\varepsilon^{3/2}}\log^{17/4}\Bigl(\frac{1}{\theta\delta^2}\Bigr) + \theta^{3/4}\Bigl(\frac{\delta+\Delta}{\varepsilon}\Bigr)^{3/2}\log^{21/4}\Bigl(\frac{1}{\theta\delta^2}\Bigr)\\&\qquad\qquad + \theta\log^3(e\theta)\Bigl(\frac{\delta+\Delta}{\varepsilon}\Bigr)^2\log^4\Bigl(\frac{1}{\theta\delta^2}\Bigr)\biggr\}. \qquad (2.5.26)\end{aligned}$$

On the other hand, if $\delta \geq \theta' - \Delta$, then an application of the global entropy bound in Kim and Samworth (2016, Theorem 4) yields

$$H_{[\,]}\big(2^{1/2}\varepsilon, \mathcal{F}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}\big) \leq H_{[\,]}(2^{1/2}\varepsilon, \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}) \lesssim \frac{1}{\varepsilon^2} \lesssim \theta\Bigl(\frac{\delta+\Delta}{\varepsilon}\Bigr)^2, \qquad (2.5.27)$$

where the final inequality follows since $\theta^{-1/2} \lesssim \theta' \leq \delta + \Delta$. We deduce from (2.5.26) and (2.5.27) that

$$\begin{aligned}&\frac{1}{\delta^2}\int_{\delta^2/2^{13}}^{\delta} H_{[\,]}^{1/2}\big(2^{1/2}\varepsilon, \mathcal{F}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}\big)\,d\varepsilon\\&\quad\lesssim m^{1/2}\biggl\{\frac{\log^{3/4}\theta + (\delta+\Delta)^{3/10}}{\delta^{7/4}}\log_+^{17/8}\Bigl(\frac{1}{\theta\delta^2}\Bigr) + \theta^{3/8}\frac{(\delta+\Delta)^{3/4}}{\delta^{7/4}}\log_+^{21/8}\Bigl(\frac{1}{\theta\delta^2}\Bigr)\\&\qquad\qquad + \theta^{1/2}\log^{3/2}(e\theta)\,\frac{\delta+\Delta}{\delta^2}\log_+^3\Bigl(\frac{1}{\delta}\Bigr)\biggr\}\\&\quad\lesssim m^{1/2}\biggl\{\frac{\log^{3/4}\theta + (\delta+\Delta)^{3/10}}{\delta^{7/4}}\log_+^{17/8}\Bigl(\frac{1}{\theta\delta^2}\Bigr) + \theta^{1/2}\log^{3/2}(e\theta)\,\frac{\delta+\Delta}{\delta^2}\log_+^3\Bigl(\frac{1}{\delta}\Bigr)\biggr\}\end{aligned}$$

for all $\delta > 0$. Therefore, setting

$$\begin{aligned}\Phi_1(\delta) &:= m^{1/2}\,(\log^{3/4}\theta)\,\delta^{-7/4}\,\log_+^{17/8}\big(1/(\theta\delta^2)\big)\\\Phi_2(\delta) &:= m^{1/2}\,(\delta+\Delta)^{3/10}\,\delta^{-7/4}\,\log_+^{17/8}\big(1/(\theta\delta^2)\big)\\\Phi_3(\delta) &:= m^{1/2}\,\theta^{1/2}\log^{3/2}(e\theta)(\delta+\Delta)\,\delta^{-2}\,\log_+^3(1/\delta)\\\Phi(\delta) &:= \Phi_1(\delta)\vee\Phi_2(\delta)\vee\Phi_3(\delta)\end{aligned}$$

for all $\delta > 0$, we conclude that there exists a universal constant $C > 0$ such that $\Psi(\delta) := C\delta^2\,\Phi(\delta) \geq \delta \vee \int_{\delta^2/2^{13}}^{\delta} H_{[\,]}^{1/2}(\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}})\,d\varepsilon$ for all such δ. Note also that Φ_1, Φ_2, Φ_3 and hence Φ are decreasing on $(0,\infty)$. Now for some universal constant $\tilde{C} \geq 1$, define

$$\begin{aligned}\delta_1 &:= \{\tilde{C}(\log^{6/7}\theta)\,(m/n)^{4/7}\log_+^{17/7}(n/\log^{3/2}\theta)\}^{1/2}\\\delta_2 &:= \{\tilde{C}(m/n)^{20/29}\log^{85/29} n + \Delta^2\}^{1/2}\\\delta_3 &:= \{\tilde{C}m\theta\log^3(e\theta)\,(m/n)\log^6 n + \Delta^2\}^{1/2}.\end{aligned}$$

Since $\delta_1^{-7/4} \leq \tilde{C}^{-7/8}(\log^{-3/4}\theta)\,(m/n)^{-1/2}\log_+^{-17/8}(n/\log^{3/2}\theta) \leq (n/\log^{3/2}\theta)^{1/2}$, it follows that $\log_+(1/\delta_1^2) \lesssim \log_+(n/\log^{3/2}\theta)$, so if $\tilde{C} \geq 1$ is chosen to be sufficiently large, then

$$C\Phi_1(\delta_1) \leq Cm^{1/2}\,(\log^{3/4}\theta)\,\delta_1^{-7/4}\log_+^{17/8}(1/\delta_1^2) \leq 2^{-19}n^{1/2}.$$

Similarly, since $\delta_k + \Delta \leq 2\delta_k$ for $k = 2,3$, it can be verified that $C\Phi_k(\delta_k) \leq 2^{-19}n^{1/2}$ for $k = 2,3$ so long as $\tilde{C} \geq 1$ is taken to be sufficiently large; see (2.5.20) in the proof of Theorem 2.2.3 for details of a similar calculation. Since Φ_1, Φ_2, Φ_3 are decreasing, we conclude that if $\delta_1, \delta_2, \delta_3$ are defined as above for some suitably large universal constant $\tilde{C} \geq 1$, then every $\delta \geq \delta_* := \delta_1 \vee \delta_2 \vee \delta_3$ satisfies

$$\delta^{-2}\,\Psi(\delta) = C\Phi(\delta) \leq C\{\Phi_1(\delta_1) \vee \Phi_2(\delta_2) \vee \Phi_3(\delta_3)\} \leq 2^{-19} n^{1/2}.$$

Thus, arguing as in the proof of Theorem 2.2.3 and recalling the derivation of (2.5.21) in particular, we can now apply van de Geer (2000, Corollary 7.5) and Lemma 2.6.1 to conclude that there exists a universal constant $c' > 0$ such that

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq \delta_*^2 + C' n^{-1} \log n = (\delta_1^2 \vee \delta_2^2 \vee \delta_3^2) + c' n^{-1} \log n,$$

which implies the bound (2.3.1). This completes the proof of the theorem in the case where $\Delta < \theta'/2$. Finally, suppose on the other hand that $\Delta \geq \theta'/2 = (32\theta)^{-1/2}$. By Theorem 2.6.2, a small modification of Kim and Samworth (2016, Theorem 5), there exists a universal constant $C' > 0$ such that $\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq C' n^{-1/2} \log n$. Observe that there exists a universal constant $\bar{c} > 0$ such that if $n \geq \bar{c}\,\theta^2 \log^2 \theta$, then $C' n^{-1/2} \log n \leq 1/(32\theta) \leq \Delta^2$, in which case the desired bound (2.3.1) follows. Otherwise, if $4 \leq n < \bar{c}\,\theta^2 \log^2 \theta$, then $n^{1/2} \log^{-5} n \leq (4^{1/2} \log^{-5} 4) \vee \{(\theta \log \theta) \log^{-5} \theta\} \lesssim \theta$, so again by Theorem 2.6.2, we conclude that

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \lesssim n^{-1/2} \log n \lesssim \theta n^{-1} \log^6 n \lesssim \theta \log^3(e\theta)(m/n) \log^6 n.$$

This completes the proof of (2.3.1) in the remaining cases. □

Next, we study the map $f_0 \mapsto \mathbb{E}\{d_X^2(\hat{f}_n, f_0)\}$ and prove the lower semi-continuity result stated as Proposition 2.3.2, for which we require the following additional definitions. We write $d_W(Q_1, Q_2) := \inf_{(X,Y)} \mathbb{E}(\|X - Y\|)$ for the *1-Wasserstein distance* between probability measures Q_1, Q_2 on $\mathbb{R}^d$, where the infimum is taken over all pairs of random variables X, Y that are defined on a common probability space and have marginal distributions Q_1, Q_2 respectively. For probability measures $Q, Q_1, Q_2, \ldots$ on $\mathbb{R}^d$, recall that $d_W(Q_n, Q) \to 0$ if and only if $Q_n \to Q$ weakly and $\int \|x\|\, dQ_n(x) \to \int \|x\|\, dQ(x)$. For $\phi \in \Phi_d$ and a probability measure Q on $\mathbb{R}^d$, we also define $L(\phi, Q) := 1 + \int \phi\, dQ - \int e^{\phi}$ and $L(Q) := \sup_{\phi \in \Phi_d} L(\phi, Q)$, as in Dümbgen et al. (2011).

Proof of Proposition 2.3.2. Since $P^{(\ell)} \to P^{(0)}$ weakly, Skorokhod's representation theorem (e.g. van der Vaart, 1998, Theorem 2.19) implies that there exist random variables $\{X^{(\ell)} : \ell \in \mathbb{N}_0\}$ defined on a common probability space $(\tilde{\Omega}, \tilde{\mathcal{A}}, \tilde{\mathbb{P}})$, with the property that $X^{(\ell)} \sim P^{(\ell)}$ for all $\ell \in \mathbb{N}_0$ and $X^{(\ell)} \to X^{(0)}$ almost surely. Now consider the n-fold product space $(\Omega, \mathcal{A}, \mathbb{P}) := (\tilde{\Omega}^n, \tilde{\mathcal{A}}^{\otimes n}, \tilde{\mathbb{P}}^{\otimes n})$, where $\tilde{\mathbb{P}}^{\otimes n}$ denotes the n-fold product measure, and for $i \in \{1, \ldots, n\}$ and $\ell \in \mathbb{N}_0$, define $X_i^{(\ell)} \colon \tilde{\Omega}^n \to \mathbb{R}^d$ by $X_i^{(\ell)}(\omega_1, \ldots, \omega_n) := X^{(\ell)}(\omega_i)$. Then for each such i, we certainly have $X_i^{(\ell)} \to X_i^{(0)}$ almost surely as $\ell \to \infty$. Moreover, if $A_1, \ldots, A_n \in \tilde{\mathcal{A}}$ and $\ell \in \mathbb{N}_0$ is fixed, then

$$\mathbb{P}\bigl(\bigcap_{i=1}^n \{X_i^{(\ell)} \in A_i\}\bigr) = \tilde{\mathbb{P}}^{\otimes n}\bigl(\prod_{i=1}^n (X^{(\ell)})^{-1}(A_i)\bigr) = \prod_{i=1}^n \tilde{\mathbb{P}}\bigl((X^{(\ell)})^{-1}(A_i)\bigr) = \prod_{i=1}^n P^{(\ell)}(A_i),$$

which shows that $X_1^{(\ell)}, \ldots, X_n^{(\ell)} \overset{\mathrm{iid}}{\sim} P^{(\ell)}$.

Next, for each $\ell \in \mathbb{N}_0$ (and $\omega \in \Omega$), denote by $\mathbb{P}_n^{(\ell)} \equiv \mathbb{P}_n^{(\ell)}(\omega) := n^{-1} \sum_{i=1}^n \delta_{X_i^{(\ell)}(\omega)}$ the empirical measure of $X_1^{(\ell)}(\omega), \ldots, X_n^{(\ell)}(\omega)$, where we write δ_x for a Dirac (point) mass at $x \in \mathbb{R}^d$. Since $X_i^{(\ell)} \to X_i^{(0)}$ almost surely for each $i \in \{1, \ldots, n\}$, there exists $\Omega_0 \in \mathcal{A}$ with $\mathbb{P}(\Omega_0) = 1$ such that whenever $\omega \in \Omega_0$ and $g \colon \mathbb{R}^d \to \mathbb{R}$ is continuous, we have

$$\int g(x)\, \mathbb{P}_n^{(\ell)}(\omega)(dx) = \frac{1}{n} \sum_{i=1}^n g\bigl(X_i^{(\ell)}(\omega)\bigr) \to \frac{1}{n} \sum_{i=1}^n g\bigl(X_i^{(0)}(\omega)\bigr) = \int g(x)\, \mathbb{P}_n^{(0)}(\omega)(dx)$$

as $\ell \to \infty$. This implies that $\int \|x\| \, \mathbb{P}_n^{(\ell)}(\omega)(dx) \to \int \|x\| \, \mathbb{P}_n^{(0)}(\omega)(dx)$ and $\mathbb{P}_n^{(\ell)}(\omega) \to \mathbb{P}_n^{(0)}(\omega)$ weakly for all $\omega \in \Omega_0$. Therefore, $d_W(\mathbb{P}_n^{(\ell)}, \mathbb{P}_n^{(0)}) \to 0$ almost surely as $\ell \to \infty$.

By assumption, $f^{(\ell)} \in \mathcal{F}_d$ for all $\ell \in \mathbb{N}$ and $P^{(0)}$ has a Lebesgue density. Since $P^{(\ell)} \to P^{(0)}$ weakly, it follows from Cule and Samworth (2010, Proposition 2) that $P^{(0)}$ has a log-concave density $f^{(0)}$ with $f^{(\ell)} \to f^{(0)}$ almost everywhere. Since replacing $f^{(0)}$ by an equivalent density alters $d_X^2(\hat{f}_n^{(0)}, f^{(0)})$ only up to almost sure equivalence, we may assume without loss of generality that $f^{(0)}$ is upper semi-continuous, i.e. that $f^{(0)} \in \mathcal{F}_d$. Therefore, the random variables $d_X^2(\hat{f}_n^{(\ell)}, f^{(\ell)}) \colon \Omega \to \mathbb{R}$ satisfy $d_X^2(\hat{f}_n^{(\ell)}, f^{(\ell)}) \geq \mathrm{KL}(\hat{f}_n^{(\ell)}, f^{(\ell)}) \geq 0$ for all $\ell \in \mathbb{N}_0$, so by Fatou's lemma, the desired conclusion will follow if we can show that

$$d_X^2(\hat{f}_n^{(\ell)}, f^{(\ell)}) = \int \log\bigl(\hat{f}_n^{(\ell)}/f^{(\ell)}\bigr) \, d\mathbb{P}_n^{(\ell)} \to \int \log\bigl(\hat{f}_n^{(0)}/f^{(0)}\bigr) \, d\mathbb{P}_n^{(0)} = d_X^2(\hat{f}_n^{(0)}, f^{(0)}) \tag{2.5.28}$$

almost surely as $\ell \to \infty$.

To this end, note that since $d_W(\mathbb{P}_n^{(\ell)}, \mathbb{P}_n^{(0)}) \to 0$ almost surely as $\ell \to \infty$, we deduce from the definition of $\hat{f}_n^{(\ell)}$ and Dümbgen et al. (2011, Theorem 2.15) that

$$\int \log \hat{f}_n^{(\ell)} \, d\mathbb{P}_n^{(\ell)} = L\bigl(\mathbb{P}_n^{(\ell)}\bigr) \to L\bigl(\mathbb{P}_n^{(0)}\bigr) = \int \log \hat{f}_n^{(0)} \, d\mathbb{P}_n^{(0)} \tag{2.5.29}$$

almost surely as $\ell \to \infty$. To establish (2.5.28), it is enough to show that $\log f^{(\ell)}\bigl(X_i^{(\ell)}\bigr) \to \log f^{(0)}\bigl(X_i^{(0)}\bigr)$ almost surely for each $i \in \{1, \ldots, n\}$, since this will imply that

$$\int \log f^{(\ell)} \, d\mathbb{P}_n^{(\ell)} = \frac{1}{n} \sum_{i=1}^n \log f^{(\ell)}\bigl(X_i^{(\ell)}\bigr) \to \frac{1}{n} \sum_{i=1}^n \log f^{(0)}\bigl(X_i^{(0)}\bigr) = \int \log f^{(0)} \, d\mathbb{P}_n^{(0)} \tag{2.5.30}$$

almost surely as $\ell \to \infty$. To this end, recall that $\phi_\ell := \log f^{(\ell)}$ is concave for each $\ell \in \mathbb{N}_0$ and that $\phi_\ell \to \phi_0$ almost everywhere. For fixed $x \in \operatorname{Int} \operatorname{dom} \phi_0$, we can find $\delta > 0$ and $w_1, \ldots, w_{d+1} \in \operatorname{Int} \operatorname{dom} \phi_0$ such that $\phi_\ell(w_k) \to \phi_0(w_k)$ for all $1 \leq k \leq d+1$ and $B(x, \delta) \subseteq \operatorname{conv}\{w_1, \ldots, w_{d+1}\} \subseteq \operatorname{Int} \operatorname{dom} \phi_0$. Then $\inf_{B(x,\delta)} \phi_\ell \geq \inf_{1 \leq k \leq d+1} \phi_\ell(w_k)$ by the concavity of ϕ_ℓ for each $\ell \in \mathbb{N}$, and since the latter quantity converges to $\inf_{1 \leq k \leq d+1} \phi_0(w_k) > -\infty$, we deduce that $B(x, \delta) \subseteq \operatorname{Int} \operatorname{dom} \phi_\ell$ for all sufficiently large $\ell \in \mathbb{N}$. Since $\phi_\ell \to \phi_0$ (almost everywhere) on $B(x, \delta) \subseteq \operatorname{Int} \operatorname{dom} \phi_0$, Rockafellar (1997, Theorem 10.8) implies that $\phi_\ell \to \phi_0$ uniformly on compact subsets of $B(x, \delta)$. In view of this and the continuity of ϕ_0 on $B(x, \delta) \subseteq \operatorname{Int} \operatorname{dom} \phi_0$ (Schneider, 2014, Theorem 1.5.3), it follows that if $x_\ell \to x$, then

$$|\phi_\ell(x_\ell) - \phi_0(x)| \leq |\phi_\ell(x_\ell) - \phi_0(x_\ell)| + |\phi_0(x_\ell) - \phi_0(x)| \to 0 \tag{2.5.31}$$

since $x_\ell \in \bar{B}(x, \delta/2)$ for all sufficiently large ℓ. Thus, writing $\Omega_0' \in \mathcal{A}$ for the event on which $X_i^{(\ell)} \to X_i^{(0)}$ and $X_i^{(0)} \in \operatorname{Int} \operatorname{dom} \phi_0 = \operatorname{Int} \operatorname{supp} f^{(0)}$ for all $i \in \{1, \ldots, n\}$, we see that $\mathbb{P}(\Omega_0') = 1$ and deduce from (2.5.31) that $\phi_\ell\bigl(X_i^{(\ell)}(\omega)\bigr) \to \phi_0\bigl(X_i^{(0)}(\omega)\bigr)$ for all $i \in \{1, \ldots, n\}$ whenever $\omega \in \Omega_0'$. This yields (2.5.30), which together with (2.5.29) implies (2.5.28), as required. □

2.5.3 Proofs of results in Section 2.4

Our first task in this section is to give the proofs of Propositions 2.4.1 and 2.4.2, which are fairly routine.

Proof of Proposition 2.4.1. For (i), fix a density $f \in \mathcal{F}^{(\beta,\Lambda,\tau)}$ and define $g \in \mathcal{F}_d$ by $g(x) := |\det A|^{-1} f\bigl(A^{-1}(x-b)\bigr)$, where $b \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$ is invertible. Since $\Sigma_g = A \Sigma_f A^\top$, we have $g(x) \det^{1/2} \Sigma_g = f\bigl(A^{-1}(x-b)\bigr) \det^{1/2} \Sigma_f$ and $\|A^{-1}x\|_{\Sigma_f} = \|x\|_{\Sigma_g}$ for all $x \in \mathbb{R}^d$. Now fix $x, y \in \mathbb{R}^d$ satisfying $g(y) < g(x) < \tau \det^{-1/2} \Sigma_g$, and let $x' := A^{-1}(x-b)$ and $y' := A^{-1}(y-b)$. Since

$f(y') < f(x') < \tau\det^{-1/2}\Sigma_f$, it follows from (2.4.1) that

$$\|x-y\|_{\Sigma_g} = \|x'-y'\|_{\Sigma_f} \geq \frac{\{f(x')-f(y')\}\det^{1/2}\Sigma_f}{\Lambda\,\{f(x')\det^{1/2}\Sigma_f\}^{1-1/\beta}} = \frac{\{g(x)-g(y)\}\det^{1/2}\Sigma_g}{\Lambda\,\{g(x)\det^{1/2}\Sigma_g\}^{1-1/\beta}}.$$

This shows that $g \in \mathcal{F}^{(\beta,\Lambda,\tau)}$, as required.

For (ii), fix $f \in \mathcal{F}^{(\beta,\Lambda,\tau)} \cap \mathcal{F}^{0,I}$ and consider $x, y \in \mathbb{R}^d$ such that $f(x) \geq \tau$ and $f(y) < f(x)$. Now let $z_t := x + t(y-x)$ and define $h(t) := -\log f(z_t)$ for $t \geq 0$, so that $h\colon [0,\infty) \to \mathbb{R}$ is continuous and convex. Then there exist unique $t_2 > t_1 \geq 0$ such that $h(t_1) = -\log\tau$, $h(t_2) = -\log\tau + \log f(x) - \log f(y)$ and h is strictly increasing on $[t_1,\infty)$. It follows from the convexity of h that $h(t_1+1)-h(t_1) \geq h(1)-h(0) = \log f(x) - \log f(y) = h(t_2)-h(t_1)$. Thus, $h(t_1+1) \geq h(t_2) > h(t_1)$ and so $0 < t_2 - t_1 \leq 1$. Since $\tau\, f(y)/f(x) = f(z_{t_2}) < f(z_{t_1}) = \tau$ and $f \leq B_d$ on $\mathbb{R}^d$, we deduce from (2.4.1) that

$$\begin{aligned}
\|x-y\| &\geq \|z_{t_1} - z_{t_2}\| \\
&\geq \Lambda^{-1}\,\frac{f(z_{t_1}) - f(z_{t_2})}{f(z_{t_1})^{1-1/\beta}} = \Lambda^{-1}\,\frac{\tau\{1-f(y)/f(x)\}}{\tau^{1-1/\beta}} = \Lambda^{-1}\left(\frac{\tau}{f(x)}\right)^{1/\beta}\frac{f(x)-f(y)}{f(x)^{1-1/\beta}} \\
&\geq \Lambda^{-1}\left(\frac{\tau}{B_d}\right)^{1/\beta}\frac{f(x)-f(y)}{f(x)^{1-1/\beta}}.
\end{aligned}$$

This shows that $\mathcal{F}^{(\beta,\Lambda,\tau)} \cap \mathcal{F}^{0,I} \subseteq \mathcal{F}^{(\beta,\Lambda^*)} \cap \mathcal{F}^{0,I}$ for all $\Lambda^* \geq \Lambda(B_d/\tau)^{1/\beta}$. Since we established in (i) that the classes $\mathcal{F}^{(\beta,\Lambda,\tau)}$ and $\mathcal{F}^{(\beta,\Lambda^*)}$ are affine invariant, the desired conclusion (ii) follows.

As for (iii), we rely on affine invariance once again in order to reduce to the isotropic case, and the result is an immediate consequence of the fact that $f \leq B_d$ on $\mathbb{R}^d$ for all $f \in \mathcal{F}^{0,I}$; indeed, for each such f, we have $\Lambda' f(x)^{1-1/\alpha} \geq \Lambda f(x)^{1-1/\beta}$ for all $x \in \mathbb{R}^d$ whenever $\Lambda' \geq B_d^{1/\alpha-1/\beta}\Lambda$.

To establish (iv), we appeal to Lovász and Vempala (2006, Theorem 5.14(c)), which asserts that $\max_{x\in\mathbb{R}^d} h(x) > (4e\pi)^{-d/2} =: t_d$ for all $h \in \mathcal{F}^{0,I}$. We also recall that there exist $\tilde{A}_d > 0$ and $\tilde{B}_d \in \mathbb{R}$, which depend only on d, such that $h(x) \leq \exp(-\tilde{A}_d\|x\| + \tilde{B}_d)$ for all $h \in \mathcal{F}^{0,I}$ and $x \in \mathbb{R}^d$ (e.g. Kim and Samworth, 2016, Theorem 2(a)). This implies that there exists $R_d > 0$, which depends only on d, such that $h(x) < t_d/2$ whenever $h \in \mathcal{F}^{0,I}$ and $\|x\| > R_d$. Now if $\beta \geq 1$ and $\Lambda > 0$ are such that $\mathcal{F}^{(\beta,\Lambda)}$ is non-empty, then by affine invariance, there must exist $f \in \mathcal{F}^{(\beta,\Lambda)} \cap \mathcal{F}^{0,I}$. By the facts above and the continuity of f, there exist $x, y \in \mathbb{R}^d$ such that $f(x) = t_d$ and $f(y) = t_d/2$. It follows from the defining condition (2.4.1) that

$$\Lambda^{-1}\,t_d/2 \leq \Lambda^{-1}\,t_d^{1/\beta}/2 = \frac{f(x)-f(y)}{\Lambda f(x)^{1-1/\beta}} \leq \|x-y\| \leq \|x\| + \|y\| \leq 2R_d$$

and hence that $\Lambda \geq R_d^{-1}\,t_d/4 =: \Lambda_{0,d}$, as required. □

Proof of Proposition 2.4.2. Throughout, we write $\Sigma \equiv \Sigma_f$ for convenience. First suppose that (2.4.2) holds for all $x \in \mathbb{R}^d$ satisfying $f(x) < \tau\det^{-1/2}\Sigma$, where $\tau \leq \tau^*\det^{1/2}\Sigma$ is fixed. Fix $x, y \in \mathbb{R}^d$ such that $f(y) < f(x) < \tau\det^{-1/2}\Sigma$, and let $t' := \inf\{t \in (0,1] : f(y + t(x-y)) = f(x)\}$. It follows from the continuity of f that $t' > 0$ and that $x' := y + t'(x-y)$ satisfies $f(x') = f(x) > 0$. Moreover, since $[y, x'] \subseteq \{w : f(w) < \tau\det^{-1/2}\Sigma_f\}$, an open set on which f is differentiable, the mean value theorem guarantees the existence of $z \in [y,x']$ such that $\nabla f(z)^\top\,\Sigma\left\{\Sigma^{-1}(x'-y)\right\} = \nabla f(z)^\top(x'-y) = f(x') - f(y) = f(x) - f(y)$. By considering the inner product $\langle v,w\rangle' := (\det\Sigma)\,(v^\top\Sigma w)$ on $\mathbb{R}^d$ that gives rise to the norm $\|\cdot\|'_{\Sigma^{-1}}$, we can apply the Cauchy–Schwarz inequality together with (2.4.2) to deduce that

$$f(x) - f(y) \le \frac{\|\nabla f(z)\|'_{\Sigma^{-1}} \, \|\Sigma^{-1}(x'-y)\|'_{\Sigma^{-1}}}{\det \Sigma} \le \frac{\Lambda \left\{ f(z) \mathrm{det}^{1/2} \Sigma \right\}^{1-1/\beta} \|x' - y\|_\Sigma}{\mathrm{det}^{1/2} \Sigma}.$$

By the choice of t', we have $f(z) \le f(x)$, so we obtain the desired conclusion that

$$\|x - y\|_\Sigma \ge \|x' - y\|_\Sigma \ge \Lambda^{-1} \frac{\{f(x) - f(y)\} \mathrm{det}^{1/2} \Sigma}{\left\{ f(x) \mathrm{det}^{1/2} \Sigma \right\}^{1-1/\beta}}.$$

Turning to the reverse implication, suppose that (2.4.1) holds whenever $x, y \in \mathbb{R}^d$ satisfy $f(y) < f(x) < \tau \mathrm{det}^{-1/2} \Sigma_f$. Now fix $x \in \mathbb{R}^d$ such that $f(x) < \tau \mathrm{det}^{-1/2} \Sigma$, which by assumption is a point at which f is differentiable, and let $u := -\Sigma \, \nabla f(x)$. It can be assumed without loss of generality that $u \neq 0$, since otherwise the desired conclusion follows trivially. Setting $h(t) := f(x + tu)$ for $t \ge 0$, we now apply the chain rule to deduce that

$$\begin{aligned} \|\nabla f(x)\|'_{\Sigma^{-1}} &= -\frac{h'(0) \mathrm{det}^{1/2} \Sigma}{\|\Sigma \, \nabla f(x)\|_\Sigma} = \lim_{t \searrow 0} \frac{\{h(0) - h(t)\} \mathrm{det}^{1/2} \Sigma}{\|tu\|_\Sigma} \\ &= \lim_{t \searrow 0} \frac{\{f(x) - f(x + tu)\} \mathrm{det}^{1/2} \Sigma}{\|tu\|_\Sigma} \le \Lambda \left\{ f(x) \mathrm{det}^{1/2} \Sigma \right\}^{1-1/\beta}, \end{aligned}$$

as required, where we have used (2.4.1) to obtain the final bound. □

Next, we establish a local bracketing entropy bound from which we will subsequently deduce our main result, Theorem 2.4.3.

Proposition 2.5.2. *Let $d = 3$ and let $\Lambda_0 \equiv \Lambda_{0,3} > 0$ be the universal constant from Proposition 2.4.1(iv). Then there exists a universal constant $\bar{c} \in (0,1)$ such that whenever $0 < \varepsilon < \delta < e^{-1} \wedge (\bar{c} \Lambda^{-3/2} \log_+^{-1} \Lambda)$ and $f_0 \in \mathcal{F}^{(\beta,\Lambda)}$ for some $\beta \ge 1$ and $\Lambda \ge \Lambda_0$, we have*

$$\begin{aligned} H_{[\,]}\bigl(2^{1/2}\varepsilon, \tilde{\mathcal{F}}(f_0, \delta) \cap \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}\bigr) \lesssim \Lambda \Biggl\{ & \frac{(\Lambda^3 \delta^2)^{(\beta-1)/(\beta+3)}}{\varepsilon^2} \log^{6(\beta+2)/(\beta+3)}(\Lambda^{-3}\delta^{-2}) \\ & + \frac{(\Lambda^3 \delta^2)^{-\frac{(4-3\beta)^+}{4(\beta+3)}}}{\varepsilon^{3/2}} \log^{(16\beta+39)/\{2(\beta+3)\}}(\Lambda^{-3}\delta^{-2}) \Biggr\}. \end{aligned} \tag{2.5.32}$$

Proof. Let $\bar{c} := e^{-1/2} \wedge \tilde{c} \wedge \tilde{c}'$, where $\tilde{c}, \tilde{c}'$ are the universal constants from Lemmas 2.8.1 and 2.8.2 respectively, and fix $0 < \varepsilon < \delta < e^{-1} \wedge (\bar{c} \Lambda^{-3/2} \log_+^{-1} \Lambda)$. Since d_{H} is affine invariant, we may assume without loss of generality that $f_0 \in \mathcal{F}^{(\beta,\Lambda)} \cap \mathcal{F}^{0,I}$. First, recall from Kim and Samworth (2016, Corollary 3(a)) that there exist universal constants $\tilde{a}_3 > 0$ and $\tilde{b}_3 \in \mathbb{R}$ such that

$$\sup_{h \in \tilde{\mathcal{F}}^{1,\eta}} h(x) \le \exp\bigl(-\tilde{a}_3 \|x\| + \tilde{b}_3\bigr) =: M(x). \tag{2.5.33}$$

for all $x \in \mathbb{R}^3$. Thus, there exists a universal constant $C_3^* > 0$ such that $f_0(x) \le M(x) \le \Lambda^3 \delta^2$ whenever $\|x\| > C_3^* \log(\Lambda^{-3}\delta^{-2})$. Now let $r := \lceil C_3^* \log(\Lambda^{-3}\delta^{-2}) \vee (2\Lambda_0 \bar{\eta})^{-1} \rceil$ and $D := [-r, r]^3$, where the universal constants $\Lambda_0 > 0$ and $\bar{\eta} \equiv \bar{\eta}_3 > 0$ are taken from Proposition 2.4.1 and Lemma 2.8.3 respectively, and observe that

$$H_{[\,]}\bigl(2^{1/2}\varepsilon, \tilde{\mathcal{F}}(f_0, \delta) \cap \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}\bigr) \le H_{[\,]}(\varepsilon, \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, D^c) + H_{[\,]}\bigl(\varepsilon, \tilde{\mathcal{F}}(f_0, \delta) \cap \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, D\bigr). \tag{2.5.34}$$

We begin by considering the first quantity on the right hand side. For each $z = (z_1, z_2, z_3) \in \mathbb{Z}^3$, let $R_z := \prod_{j=1}^3 [z_j, z_j + 1)$ and note that $m_z := \max_{y \in R_z} M(y) \leq e^{\sqrt{3}\tilde{a}_3} M(w)$ for all $w \in R_z$. Writing $A \triangle B$ for the symmetric difference of sets A, B, we set $J := \{z \in \mathbb{Z}^3 : R_z \not\subseteq D\}$ and observe that $\mu_3\bigl(D^c \triangle \bigcup_{z \in J} R_z\bigr) = 0$, from which we deduce that

$$
\begin{aligned}
b := \sum_{z \in J} m_z^{1/2} \leq e^{\sqrt{3}\tilde{a}_3/2} \int_{D^c} M^{1/2} \leq e^{\sqrt{3}\tilde{a}_3/2} \int_{\bar{B}(0,r)^c} M^{1/2} = 4\pi e^{\sqrt{3}\tilde{a}_3/2} \int_r^\infty t^2 e^{-(\tilde{a}_3 t - \tilde{b}_3)/2}\, dt \\
\lesssim \Lambda^{3/2} \delta \log^2(\Lambda^{-3}\delta^{-2}). \qquad (2.5.35)
\end{aligned}
$$

We now apply the bound (2.6.35) from Proposition 2.6.7 to establish that

$$
\begin{aligned}
H_{[\,]}(\varepsilon, \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, D^c) &\leq \sum_{z \in J} H_{[\,]}(m_z^{1/4} b^{-1/2} \varepsilon, \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, R_z) \\
&\lesssim \sum_{z \in J} \frac{m_z^{1/2}}{b^{-1}\varepsilon^2} \lesssim \frac{\Lambda^3 \delta^2 \log^4(\Lambda^{-3}\delta^{-2})}{\varepsilon^2}. \qquad (2.5.36)
\end{aligned}
$$

To handle the second term on the right hand side of (2.5.34), we subdivide D further into regions that are derived from polytopal approximations to the closed, convex sets defined by $U_{f_0,t} := \{x \in \mathbb{R}^d : f_0(x) \geq t\}$ for $t \geq 0$. We start by making some further definitions. Let $\ell := (\tilde{c}\Lambda^3\delta^2)^{\beta/(\beta+3)}$, where $\tilde{c} > 1$ is the universal constant defined in Lemma 2.8.1. Since $\delta < \bar{c}\Lambda^{-3/2}\log_+^{-1}\Lambda$ and $\bar{c} < 1$, we have $\Lambda^3\delta^2 < 1$, so $\ell \geq \tilde{c}^{\beta/(\beta+3)}\Lambda^3\delta^2 > \Lambda^3\delta^2$. Also, by Lovász and Vempala (2006, Theorem 5.14(c)) and the proof of Kim and Samworth (2016, Corollary 3(b)), we have $\inf_{h \in \tilde{\mathcal{F}}^{1,\eta}} \sup_{x \in \mathbb{R}^d} h(x) > (1+\eta)^{-3/2}(4e\pi)^{-3/2} =: t_0$, and note that $k_0 := \lfloor \log_2(t_0\,\ell^{-1}) \rfloor \lesssim \log(\Lambda^{-3}\delta^{-2})$.

Now for $k \in \{0, \ldots, k_0\}$, define $U_k := U_{f_0,\,2^k\ell}$ and $r_k := (2\Lambda)^{-1}(2^k\ell)^{1/\beta}$. Then $r_k \leq r_{k_0} \leq (2\Lambda)^{-1}t_0^{1/\beta} \leq (2\Lambda)^{-1}$ for all such k. Recalling the definition of r and the fact that $\ell > \Lambda^3\delta^2$, we see that $D \supseteq \bar{B}(0,r) \supseteq U_{f_0,\,\Lambda^3\delta^2} \supseteq U_0 \supseteq U_1 \supseteq \cdots \supseteq U_{k_0} \supseteq U_{f_0,\,t_0} \neq \emptyset$. Also, since f satisfies (2.4.1), it follows that $U_{k-1} \supseteq U_k + \bar{B}(0, r_k)$ for every $k \in \{1, \ldots, k_0\}$.

Next, we obtain suitable approximating polytopes $P_0 \supseteq \cdots \supseteq P_{k_0-1}$. For each fixed $k \in \{1, \ldots, k_0\}$, note that $r_k/r \leq (2\Lambda)^{-1}/(2\Lambda_0\bar{\eta})^{-1} \leq \bar{\eta}$ in view of the definition of r, and that $U_k \subseteq \bar{B}(0,r)$ is compact and convex. Thus, by Lemma 2.8.3, there exists a polytope P_{k-1} with at most $\bar{C}^*(r_k/r)^{-1} \lesssim (2^k\ell)^{-1/\beta}\Lambda\log(\Lambda^{-3}\delta^{-2})$ vertices such that $U_k \subseteq P_{k-1} \subseteq U_k + \bar{B}(0, r_k) \subseteq U_{k-1}$. We emphasise that the hidden constant here does not depend on k. In addition, let $P_{k_0} := \emptyset$.

In the argument below, we also use the fact that if $P \subseteq Q \subseteq \mathbb{R}^3$ are polytopes with p and q vertices respectively, then there is a triangulation of $Q \setminus \operatorname{Int} P$ containing $\lesssim p + q$ simplices (Wang and Yang, 2000). We will apply this to the nested pairs $P_0 \subseteq D$ and $P_k \subseteq P_{k-1}$ for $1 \leq k \leq k_0$.

First, we consider the region $D \setminus P_0$. By the facts above, $D \setminus \operatorname{Int} P_0$ can be triangulated into $\lesssim \ell^{-1/\beta}\Lambda\log(\Lambda^{-3}\delta^{-2})$ simplices. Also, since $U_1 \subseteq P_0$, we have $f_0(x) \leq 2\ell$ for all $x \in D \setminus P_0$. Thus, by Lemma 2.8.2 and the fact that $\ell \asymp (\Lambda^3\delta^2)^{\beta/(\beta+3)}$, each $f \in \tilde{\mathcal{F}}(f_0, \delta) \cap \tilde{\mathcal{F}}^{1,\eta}$ satisfies $f \lesssim \ell \log^{2\beta/(\beta+3)}(\Lambda^{-3}\delta^{-2})$ on $D \setminus P_0$. We now apply the final assertion of Proposition 2.6.7 together with the bound $\mu_3(D \setminus P_0) \leq \mu_3(D) \lesssim \log^3(\Lambda^{-3}\delta^{-2})$ to deduce that

$$
\begin{aligned}
&H_{[\,]}\bigl(2^{-1/2}\varepsilon, \tilde{\mathcal{F}}(f_0,\delta) \cap \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, D \setminus P_0\bigr) \\
&\quad\lesssim \ell^{-1/\beta}\Lambda\log(\Lambda^{-3}\delta^{-2})\, \frac{\ell \log^{2\beta/(\beta+3)}(\Lambda^{-3}\delta^{-2}) \log^3(\Lambda^{-3}\delta^{-2})}{\varepsilon^2} \\
&\quad\lesssim \Lambda\, \frac{(\Lambda^3\delta^2)^{(\beta-1)/(\beta+3)}}{\varepsilon^2} \log^{6(\beta+2)/(\beta+3)}(\Lambda^{-3}\delta^{-2}). \qquad (2.5.37)
\end{aligned}
$$

Next, fix $1 \leq k \leq k_0$ and consider $P_{k-1} \setminus P_k$. By the facts above, $P_{k-1} \setminus \operatorname{Int} P_k$ can be triangulated into $\lesssim (2^k\ell)^{-1/\beta}\Lambda\log(\Lambda^{-3}\delta^{-2})$ simplices. Moreover, since $P_{k-1} \setminus P_k \subseteq U_{k-1} \setminus U_{k+1}$, we have

$2^{k-1}\ell \le f_0(x) < 2^{k+1}\ell$ for all $x \in P_{k-1} \setminus P_k$. Thus, by the choice of $\bar{c}$ at the start of the proof and the fact that $\ell \asymp (\Lambda^3\delta^2)^{\beta/(\beta+3)}$, it follows from Lemmas 2.8.1 and 2.8.2 that

$$2^{k-2}\ell \le f(x) \lesssim 2^k \ell \log^{2\beta/(\beta+3)}(\Lambda^{-3}\delta^{-2})$$

whenever $f \in \tilde{\mathcal{F}}(f_0,\delta) \cap \tilde{\mathcal{F}}^{1,\eta}$ and $x \in P_{k-1} \setminus P_k$. In addition, $\mu_3(P_{k-1}\setminus P_k) \le \mu_3(D) \lesssim \log^3(\Lambda^{-3}\delta^{-2})$, so by applying the first bound (2.6.33) from Proposition 2.6.7, we conclude that

$$\begin{aligned} &H_{[\,]}\bigl(\varepsilon/\sqrt{2k_0}, \tilde{\mathcal{F}}(f_0,\delta) \cap \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, P_{k-1}\setminus P_k\bigr) \\ &\qquad \lesssim (2^k\ell)^{-1/\beta}\Lambda \log(\Lambda^{-3}\delta^{-2}) \left(\frac{(2^k\ell)^{1/2}\log^{\beta/(\beta+3)}(\Lambda^{-3}\delta^{-2})\log^{5/2}(\Lambda^{-3}\delta^{-2})}{k_0^{-1/2}\,\varepsilon} \right)^{3/2} \\ &\qquad \lesssim \Lambda\, \frac{(2^k\ell)^{3/4-1/\beta}}{\varepsilon^{3/2}} \log^{(14\beta+33)/\{2(\beta+3)\}}(\Lambda^{-3}\delta^{-2}), \end{aligned} \tag{2.5.38}$$

where we emphasise again that the hidden constant here does not depend on k. Now for any $\alpha \in \mathbb{R}$, we have the simple bound $\sum_{k=0}^{k_0}(2^k\ell)^{-\alpha} \le \ell^{-\alpha^+} k_0 \lesssim \ell^{-\alpha^+}\log(\Lambda^{-3}\delta^{-2})$. Since $P_0 = \bigcup_{k=1}^{k_0}(P_{k-1}\setminus P_k)$, it follows from the above that

$$\begin{aligned} H_{[\,]}\bigl(2^{-1/2}\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, P_0\bigr) &\le \sum_{k=1}^{k_0} H_{[\,]}\bigl(\varepsilon/\sqrt{2k_0}, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, P_{k-1}\setminus P_k\bigr) \\ &\lesssim \Lambda\, \frac{(\Lambda^3\delta^2)^{-\frac{(4-3\beta)^+}{4(\beta+3)}}}{\varepsilon^{3/2}} \log^{(16\beta+39)/\{2(\beta+3)\}}(\Lambda^{-3}\delta^{-2}). \end{aligned} \tag{2.5.39}$$

Finally, since

$$\begin{aligned} H_{[\,]}\bigl(\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, D\bigr) \le{}& H_{[\,]}\bigl(2^{-1/2}\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, D\setminus P_0\bigr) \\ &+ H_{[\,]}\bigl(2^{-1/2}\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}, P_0\bigr), \end{aligned}$$

we can combine the bounds (2.5.34), (2.5.36), (2.5.37) and (2.5.39) to obtain the desired local bracketing entropy bound (2.5.32). □

Theorem 2.4.3 now follows from Proposition 2.5.2 and standard empirical process theory in much the same way that Theorem 2.2.3 follows from Proposition 2.5.1.

Proof of Theorem 2.4.3. Fix $f_0 \in \mathcal{F}_3$, $\beta \ge 1$ and $\Lambda \ge \Lambda_0$, and let $\tilde{\Delta} := \inf_{f\in\mathcal{F}_3^{(\beta,\Lambda)}} d_{\mathrm{H}}^2(f_0,f)$. Defining the universal constant $\bar{c} \in (0,1)$ as in Proposition 2.5.2, we first suppose that $\tilde{\Delta} < 2^{-1}\{e^{-1} \wedge (\bar{c}\Lambda^{-3/2}\log_+^{-1}\Lambda)\} =: 2^{-1}\tilde{\Lambda}$. If $\delta \in (0, \tilde{\Lambda} - \tilde{\Delta})$, then by analogy with the derivation of (2.5.17) in the proof of Theorem 2.2.3, we deduce from Proposition 2.5.2 and the triangle inequality that

$$\begin{aligned} H_{[\,]}\bigl(2^{1/2}\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}\bigr) \lesssim \Lambda \biggl\{ & \frac{\{\Lambda^3(\delta+\tilde{\Delta})^2\}^{\alpha}}{\varepsilon^2}\log^{\gamma}(\Lambda^{-3}\delta^{-2}) \\ &+ \frac{\{\Lambda^3(\delta+\tilde{\Delta})^2\}^{-\tilde{\alpha}}}{\varepsilon^{3/2}}\log^{\tilde{\gamma}}(\Lambda^{-3}\delta^{-2}) \biggr\}, \end{aligned} \tag{2.5.40}$$

where we set $\alpha := (\beta-1)/(\beta+3)$, $\gamma := 6(\beta+2)/(\beta+3)$, $\tilde{\alpha} := -(4-3\beta)^+/\{4(\beta+3)\}$ and $\tilde{\gamma} := (16\beta+39)/\{2(\beta+3)\}$. Since $\Lambda^{-3} \leq \Lambda_0^{-3} \lesssim 1$ and $1+\gamma/2 \leq \tilde{\gamma}/2$, it follows from (2.5.40) that

$$\begin{aligned}
&\frac{1}{\delta^2}\int_{\delta^2/2^{13}}^{\delta} H_{[\,]}^{1/2}\bigl(2^{1/2}\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}\bigr)\,d\varepsilon \\
&\quad\lesssim \frac{\Lambda^{1/2}}{\delta^2}\bigl\{\Lambda^3(\delta+\tilde{\Delta})^2\bigr\}^{\alpha/2}\log^{\gamma/2}(\Lambda^{-3}\delta^{-2})\log(1/\delta) + \frac{\Lambda^{1/2}}{\delta^{7/4}}\bigl\{\Lambda^3(\delta+\tilde{\Delta})^2\bigr\}^{-\tilde{\alpha}/2}\log^{\tilde{\gamma}/2}(\Lambda^{-3}\delta^{-2}) \\
&\quad\lesssim \log^{\tilde{\gamma}/2}(1/\delta)\left(\frac{\Lambda^{1/2}}{\delta^2}\bigl\{\Lambda^3(\delta+\tilde{\Delta})^2\bigr\}^{\alpha/2} + \frac{\Lambda^{1/2}}{\delta^{7/4}}\bigl\{\Lambda^3(\delta+\tilde{\Delta})^2\bigr\}^{-\tilde{\alpha}/2}\right) =: \Phi_1(\delta)
\end{aligned}$$

for all $\delta \in (0, \tilde{\Lambda}-\tilde{\Delta})$. Setting $\tilde{\delta} := \Lambda^3\delta^2$, observe that since

$$r_\beta^{-1} = (2-\alpha)\vee(\tilde{\alpha}+7/4) = \begin{cases} 2-\alpha = (\beta+7)/(\beta+3) & \text{if } \alpha < 1/4 \\ 7/4 & \text{if } \alpha \geq 1/4 \end{cases}$$

and $\Lambda^{25/8} \leq \Lambda_0^{-3/8}\Lambda^{7/2}$, we have

$$\begin{aligned}
\Phi_1(\delta) &\leq 2\log^{\tilde{\gamma}/2}(\Lambda^{3/2}\tilde{\delta}^{-1})\bigl(\Lambda^{7/2}\,\tilde{\delta}^{\alpha-2} + \Lambda^{25/8}\,\tilde{\delta}^{-(\tilde{\alpha}+7/4)}\bigr) \\
&\leq 2\bigl(1+\Lambda_0^{-3/8}\bigr)\Lambda^{7/2}\,\tilde{\delta}^{-1/r_\beta}\log^{\tilde{\gamma}/2}(\Lambda^{3/2}\tilde{\delta}^{-1})
\end{aligned} \tag{2.5.41}$$

for all $\delta \in (\tilde{\Delta}, \tilde{\Lambda}-\tilde{\Delta})$. On the other hand, if $\delta \geq \tilde{\Lambda}-\tilde{\Delta} > \tilde{\Lambda}/2$, then by Kim and Samworth (2016, Theorem 4), we have

$$H_{[\,]}\bigl(2^{1/2}\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}\bigr) \leq H_{[\,]}(2^{1/2}\varepsilon, \tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}) \lesssim \frac{1}{\varepsilon^2} \lesssim \frac{(\delta+\tilde{\Delta})^2}{\tilde{\Lambda}^2\,\varepsilon^2} \lesssim \frac{(\delta+\tilde{\Delta})^2\,\Lambda^3\log_+^2\Lambda}{\varepsilon^2},$$

so

$$\frac{1}{\delta^2}\int_{\delta^2/2^{13}}^{\delta} H_{[\,]}^{1/2}\bigl(2^{1/2}\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}}\bigr)\,d\varepsilon \lesssim \frac{\delta+\tilde{\Delta}}{\delta^2}\log_+\left(\frac{1}{\delta}\right)\Lambda^{3/2}\log_+^2\Lambda =: \Phi_2(\delta)$$

for all $\delta \geq \tilde{\Lambda}-\tilde{\Delta}$. It is straightforward to verify that Φ_1 and Φ_2 are decreasing functions of δ. Moreover, since $\tilde{\Lambda}/2 < \tilde{\Lambda}-\tilde{\Delta} \leq \tilde{\Lambda}$, we see that $\Phi_1(\delta) \gtrsim \Lambda^{7/2}\log_+^{2+\tilde{\gamma}/2}\Lambda$ for all $\delta \in (0, \tilde{\Lambda}-\tilde{\Delta})$ and $\Phi_2(\delta) \lesssim \Lambda^3\log_+^3\Lambda$ for all $\delta \geq \tilde{\Lambda}-\tilde{\Delta}$. Consequently, there exist universal constants $\tilde{C}', \tilde{C}'' > 0$ such that the function $\Psi\colon (0,\infty)\to(0,\infty)$ defined by

$$\Psi(\delta) := \begin{cases} \tilde{C}'\delta^2\,\Phi_1(\delta) & \text{if } \delta \in (0, \tilde{\Lambda}-\tilde{\Delta}) \\ \tilde{C}''\delta^2\,\Phi_2(\delta) & \text{if } \delta \geq \tilde{\Lambda}-\tilde{\Delta} \end{cases}$$

satisfies $\Psi(\delta) \geq \delta \vee \int_{\delta^2/2^{13}}^{\delta} H_{[\,]}^{1/2}(\varepsilon, \tilde{\mathcal{F}}(f_0,\delta)\cap\tilde{\mathcal{F}}^{1,\eta}, d_{\mathrm{H}})\,d\varepsilon$ for all $\delta > 0$ and has the property that $\delta \mapsto \delta^{-2}\,\Psi(\delta)$ is decreasing. Next, let $\tilde{C} := \Lambda_0^{-1}(1\vee\Lambda_0^{1/2}) \vee \bigl\{2^{20}\tilde{C}'\bigl(1+\Lambda_0^{-3/8}\bigr)\bigr\}^{2r_\beta}$, which satisfies $\tilde{C}\Lambda^{7r_\beta-3} \geq \tilde{C}\Lambda_0^{7r_\beta-3} \geq 1$ in view of the fact that $r_\beta \in (1/2, 4/7]$, and define

$$\delta_n := \bigl(\tilde{C}\Lambda^{7r_\beta-3}n^{-r_\beta}\log^{\tilde{\gamma}r_\beta} n + \tilde{\Delta}^2\bigr)^{1/2}.$$

It is straightforward to verify that there exists a universal constant $\tilde{K} > 1$ such that $\bar{\delta}_n := (\tilde{C}\Lambda^{7r_\beta-3}n^{-r_\beta}\log^{\tilde{\gamma}r_\beta} n)^{1/2} \leq \tilde{\Lambda}/2 < \tilde{\Lambda}-\tilde{\Delta}$ for all $n \geq \lceil\tilde{K}\Lambda^8\rceil$. Since $\delta_n > \tilde{\Delta}$ and $\log(1/\bar{\delta}_n) \leq \log n$, it follows from (2.5.41) that for all $n \geq \tilde{K}\Lambda^8$, we have

$$\begin{aligned}\delta_n^{-2}\,\Psi(\delta_n) &\leq \bar{\delta}_n^{-2}\,\Psi(\bar{\delta}_n) = \tilde{C}'\,\Phi_1(\bar{\delta}_n)\\ &\leq 2\tilde{C}'\big(1+\Lambda_0^{-3/8}\big)\Lambda^{7/2}\big(\tilde{C}^{-1}\Lambda^{-7r_\beta}n^{r_\beta}\log^{-\tilde{\gamma}r_\beta} n\big)^{1/(2r_\beta)}\log^{\tilde{\gamma}/2} n\\ &\leq 2^{-19}n^{1/2}.\end{aligned}$$

Thus, arguing as in the proof of Theorem 2.2.3 and recalling the derivation of (2.5.21) in particular, we can now apply van de Geer (2000, Corollary 7.5) and Lemma 2.6.1 to conclude that there exists a universal constant $\tilde{C}^* > 0$ such that

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq \tilde{C}^*\Lambda^{7r_\beta-3}n^{-r_\beta}\log^{\tilde{\gamma}r_\beta} n + \tilde{\Delta}^2$$

for all $n \geq \tilde{K}\Lambda^8$, provided that $\tilde{\Delta} < \tilde{\Lambda}/2$.

Suppose on the other hand that $\tilde{\Delta} \geq \tilde{\Lambda}/2$. By Theorem 2.6.2, a small modification of Kim and Samworth (2016, Theorem 5), there exists a universal constant $C' > 0$ such that $\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq C'n^{-1/2}\log n$, and observe that there exists a universal constant $K' \geq \tilde{K}$ such that if $n \geq K'\Lambda^8$ then

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \leq C'n^{-1/2}\log n \leq \{e^{-2} \wedge (\bar{c}^2\Lambda^{-3}\log_+^{-2}\Lambda)\}/4 = \tilde{\Lambda}^2/4 \leq \tilde{\Delta}^2.$$

Otherwise, if $4 \leq n < K'\Lambda^8$ and $\tilde{\Delta} \geq 0$, then since $8(r_\beta - 1/2) \leq 7r_\beta - 3$, it again follows from Theorem 2.6.2 that

$$\mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} \lesssim n^{-1/2}\log n \lesssim \Lambda^{7r_\beta-3}n^{-r_\beta}\log^{\tilde{\gamma}r_\beta} n.$$

This completes the proof of the oracle inequality (2.4.3). □

This concludes Section 2.5. We now describe the organisation of the rest of the chapter. Section 2.6.3 contains the supporting results that are most directly relevant to the proofs of the main theorems in Sections 2.2 and 2.3. Much of the groundwork for Section 2.6.3 is laid in Section 2.7.2, where many of the technical lemmas have a strong geometric flavour. The structural results in Section 2.7.1 are rooted in convex analysis and underpin many of the key definitions and calculations in Sections 2.2 and 2.5.1. Other supplementary results of a more statistical nature may be found in Sections 2.6.1 and 2.6.2 (such the envelope result stated as Proposition 2.6.3, which may be of interest in its own right).

The technical preparation for the proof of the main result in Section 2.4 is carried out in Section 2.8.1, in which the key auxiliary results play a similar role to those in Section 2.7.2. Two of the examples in Section 2.4 draw on the background material in Section 2.8.2, which develops a notion of affine invariant smoothness and reviews some existing results on nonparametric density estimation over Hölder classes.

2.6 Supplementary proofs for Sections 2.5.1 and 2.5.2

2.6.1 Tail bounds for d_X^2 divergence and their consequences

Lemma 2.6.1. *Fix $d \in \mathbb{N}$. Let $X_1, \ldots, X_n \overset{\text{iid}}{\sim} f_0 \in \mathcal{F}_d$ with $n \geq d+1$ and let $\hat{f}_n$ denote the corresponding log-concave maximum likelihood estimator. Then*

$$\mathbb{E}\left\{\sup_{x\in\mathbb{R}^d}\log\hat{f}_n(x) + \max_{i=1,\ldots,n}\log\frac{1}{f_0(X_i)}\right\} \lesssim_d \log n, \tag{2.6.1}$$

and

$$\int_{8d\log n}^{\infty} \mathbb{P}\{d_X^2(\hat{f}_n, f_0) \geq t\}\, dt \lesssim_d n^{-3}. \tag{2.6.2}$$

Proof. The case $d = 1$ of this result was proved in Lemma 2 in the online supplement to Kim et al. (2018), so suppose now that $d \geq 2$. Let $T\colon \mathbb{R}^d \to \mathbb{R}^d$ be the invertible affine transformation defined by $T(x) := \Sigma_{f_0}^{1/2} x + \mu_{f_0}$ for all $x \in \mathbb{R}^d$, and let $Y_i := T^{-1}(X_i)$ for all $i = 1, \ldots, n$. Setting $g_0(x) := f_0\bigl(T(x)\bigr)\det^{1/2}\Sigma_{f_0}$ for all $x \in \mathbb{R}^d$, we have $Y_1, \ldots, Y_n \overset{\mathrm{iid}}{\sim} g_0 \in \mathcal{F}_d^{0,I}$, and

$$\max_{i=1,\ldots,n} \log \frac{1}{g_0(Y_i)} = \max_{i=1,\ldots,n} \log \frac{1}{f_0(X_i)} - \log \det^{1/2}\Sigma_{f_0}.$$

Also, by the affine equivariance of the log-concave maximum likelihood estimator (Dümbgen et al., 2011, Remark 2.4), the corresponding $\hat{g}_n$ based on $Y_1, \ldots, Y_n$ is given by $\hat{g}_n(x) := \hat{f}_n\bigl(T(x)\bigr)\det^{1/2}\Sigma_{f_0}$ for all $x \in \mathbb{R}^d$, so

$$\sup_{x\in\mathbb{R}^d} \log \hat{g}_n(x) = \sup_{x\in\mathbb{R}^d} \log \hat{f}_n(x) + \log\det^{1/2}\Sigma_{f_0}.$$

It follows that

$$\sup_{x\in\mathbb{R}^d} \log \hat{g}_n(x) + \max_{i=1,\ldots,n} \log \frac{1}{g_0(Y_i)} = \sup_{x\in\mathbb{R}^d} \log \hat{f}_n(x) + \max_{i=1,\ldots,n} \log \frac{1}{f_0(X_i)},$$

and a similar argument shows that $d_X^2(\hat{f}_n, f_0) = d_X^2(\hat{g}_n, g_0)$, i.e. that d_X^2 is affine invariant. Therefore, for the purposes of establishing (2.6.1) and (2.6.2), there is no loss of generality in assuming henceforth that $f_0 \in \mathcal{F}_d^{0,I}$.

To begin with, we control the first term on the left hand side of (2.6.1). Write $\hat{\Sigma}_n := n^{-1}\sum_{i=1}^n (X_i - \bar{X})(X_i - \bar{X})^\top$ for the sample covariance matrix, where $\bar{X} := n^{-1}\sum_{i=1}^n X_i$, and let $\lambda_{\min}(\hat{\Sigma}_n)$ and $\lambda_{\max}(\hat{\Sigma}_n)$ denote the smallest and largest eigenvalues of $\hat{\Sigma}_n$ respectively. By the affine equivariance of the log-concave maximum likelihood estimator, together with straightforward modifications of arguments in the proof of Lemma 2 in the online supplement to Kim et al. (2018), there exists $\tilde{C}_d > 0$, depending only on d, such that for every $t > 0$,

$$\mathbb{P}\biggl(\sup_{x\in\mathbb{R}^d} \log \hat{f}_n(x) > \frac{t}{2}\log n\biggr) \leq \mathbb{P}\bigl(\det\hat{\Sigma}_n \leq \tilde{C}_d n^{-t/2}\bigr) \leq \mathbb{P}\bigl(\lambda_{\min}(\hat{\Sigma}_n) \leq \tilde{C}_d^{1/d} n^{-t/(2d)}\bigr).$$

To handle the final expression above, we now seek an upper bound on $\mathbb{P}\bigl(\lambda_{\min}(\hat{\Sigma}_n) \leq s\bigr)$ for each $s > 0$. To this end, let $\mathcal{N} \equiv \mathcal{N}(s^2/2) \subseteq S^{d-1}$ be an $(s^2/2)$-net of $S^{d-1} := \{x \in \mathbb{R}^d : \|x\| \leq 1\}$ of cardinality $K_d\, s^{-2(d-1)}$, say, where $K_d > 0$ depends only on d. Then for each $u \in S^{d-1}$, there exists $\tilde{u} \in \mathcal{N}$ such that $\|u - \tilde{u}\| \leq s^2/2$, whence

$$-s^2\lambda_{\max}(\hat{\Sigma}_n) \leq u^\top\hat{\Sigma}_n u - \tilde{u}^\top\hat{\Sigma}_n\tilde{u} = \tilde{u}^\top\hat{\Sigma}_n(u - \tilde{u}) + (u - \tilde{u})^\top\hat{\Sigma}_n u \leq s^2\lambda_{\max}(\hat{\Sigma}_n). \tag{2.6.3}$$

In particular, if $\mathcal{N}'$ is a $(1/4)$-net of S^{d-1} of cardinality $\tilde{K_d} := 2^{d-1}K_d$, then setting $s = 1/\sqrt{2}$ and taking $u \in S^{d-1}$ to be a unit eigenvector of $\hat{\Sigma}_n$ with corresponding eigenvalue $\lambda_{\max}(\hat{\Sigma}_n)$, we deduce from (2.6.3) that

$$\max_{u\in\mathcal{N}'} u^\top\hat{\Sigma}_n u \geq \frac{1}{2}\max_{u\in S^{d-1}} u^\top\hat{\Sigma}_n u = \frac{1}{2}\lambda_{\max}(\hat{\Sigma}_n). \tag{2.6.4}$$

Next, fix $\tilde{u} \in S^{d-1}$ and let $Y := (Y_1, \ldots, Y_n)$, where $Y_i := \tilde{u}^\top X_i$ for $i = 1, \ldots, n$. Also, let $Q \in \mathbb{R}^{n\times n}$ be an orthogonal matrix such that $Q_{nj} = n^{-1/2}$ for all $j = 1, \ldots, n$, and define $Z := QY$ and $W := (Z_1, \ldots, Z_{n-1})$. Then Y has an isotropic log-concave density, so the same is true of Z and W. Writing f_W for the density of W, we deduce from Lovász and Vempala (2006, Theorem 5.14(e)) that

$f_W \leq \{2^{16}(n-1)\}^{(n-1)/2}$. Moreover, setting $\bar{Y} := \tilde{u}^\top \bar{X}$, we have

$$n(\tilde{u}^\top \hat{\Sigma}_n \tilde{u}) = \sum_{i=1}^n (Y_i - \bar{Y})^2 = \|Y\|^2 - n\bar{Y}^2 = \|Z\|^2 - Z_n^2 = \|W\|^2.$$

Thus, for all $a > 0$, it follows that

$$\begin{aligned} \mathbb{P}\big(\tilde{u}^\top \hat{\Sigma}_n \tilde{u} \leq a\big) &= \mathbb{P}\big(\|W\|^2 \leq na\big) = \int_{\bar{B}(0,n^{1/2}a^{1/2})} f_W(w)\,dw \\ &\leq \{2^{16}(n-1)\}^{(n-1)/2}\,\mu_{n-1}\big(\bar{B}(0,n^{1/2}a^{1/2})\big) \leq \frac{(2^{16}\pi n^2 a)^{(n-1)/2}}{\Gamma\big((n+1)/2\big)}, \end{aligned} \tag{2.6.5}$$

where we have used the fact that $\mu_{n-1}(\bar{B}(0,r)) = (\pi^{1/2}r)^{n-1}/\Gamma\big((n+1)/2\big)$ for all $r > 0$. Furthermore, by Guédon and Milman (2011, Theorem 1.1), there exist universal constants $C, c > 0$ such that for all $b > 0$, we have

$$\begin{aligned} \mathbb{P}\big(\tilde{u}^\top \hat{\Sigma}_n \tilde{u} > b\big) &\leq \mathbb{P}\left(\sum_{i=1}^n (\tilde{u}^\top X_i)^2/n > b\right) \\ &\leq C\exp\left(-cn^{1/2}\min\left\{n^{3/2}(b^{1/2}-1)^3, n^{1/2}(b^{1/2}-1)\right\}\right), \end{aligned} \tag{2.6.6}$$

which is at most $C\exp\big(-cn(b^{1/2}-1)\big) \leq C\exp(-cnb^{1/2}/2)$ when $b \geq 4$. Now let $s := \tilde{C}_d^{1/d} n^{-t/(2d)}$, and for this value of s, let $\mathcal{N}$ be an $(s^2/2)$-net of S^{d-1}. Then taking $a = 2s$ and $b = (2s)^{-1}$ in (2.6.5) and (2.6.6) respectively, we deduce that

$$\begin{aligned} &\mathbb{P}\left(\sup_{x\in\mathbb{R}^d} \log \hat{f}_n(x) > \frac{t}{2}\log n\right) \\ &\leq \mathbb{P}\big(\lambda_{\min}(\hat{\Sigma}_n) \leq s\big) = \mathbb{P}\left(\inf_{u\in S^{d-1}} u^\top \hat{\Sigma}_n u \leq s\right) \\ &\leq \mathbb{P}\left(\min_{u\in\mathcal{N}} u^\top \hat{\Sigma}_n u - s^2\lambda_{\max}(\hat{\Sigma}_n) \leq s\right) \leq \mathbb{P}\left(\min_{u\in\mathcal{N}} u^\top \hat{\Sigma}_n u \leq 2s\right) + \mathbb{P}\big(\lambda_{\max}(\hat{\Sigma}_n) > s^{-1}\big) \\ &\leq \mathbb{P}\left(\min_{u\in\mathcal{N}} u^\top \hat{\Sigma}_n u \leq 2s\right) + \mathbb{P}\left(\max_{u\in\mathcal{N}'} u^\top \hat{\Sigma}_n u > (2s)^{-1}\right) \\ &\leq K_d\,\tilde{C}_d^{-2(d-1)/d} n^{t(d-1)/d}\,\frac{(2^{16}\pi)^{(n-1)/2}}{\Gamma\big((n+1)/2\big)} n^{n-1}\big(2\tilde{C}_d^{1/d} n^{-t/(2d)}\big)^{(n-1)/2} &\quad (2.6.7) \\ &\quad + \tilde{K}_d\,C\exp\left(-cn^{1/2}\min\left\{n^{3/2}(\tilde{C}_d^{-1/(2d)} n^{t/(4d)} - 1)^3, n^{1/2}(\tilde{C}_d^{-1/(2d)} n^{t/(4d)} - 1)\right\}\right), &\quad (2.6.8) \\ &=: R_1 + R_2, \end{aligned}$$

where the second, fourth and fifth inequalities follow from (2.6.3), (2.6.4) and a union bound respectively. We now consider R_1 and R_2 separately. Setting $\zeta_d := (d+1) \vee 2^{17}\tilde{C}_d^{1/d}\pi$, note that we can find $n_d > \zeta_d$ depending only on d such that

$$\zeta_d^{(n-1)/2} n^{n-1} \int_{8d}^\infty n^{t\,(\frac{d-1}{d} - \frac{n-1}{4d})}\,dt \leq \zeta_d^{(n-1)/2} n^{n-1}\, n^{8d\,(\frac{d-1}{d} - \frac{n-1}{4d})} \leq n^{-n/2} \tag{2.6.9}$$

for all $n \geq n_d$. This takes care of R_1. Also, $\tilde{C}_d^{-1/d} n^{t/(2d)} \geq 4$ whenever $t \geq 4d$ and $n \geq n_d > 2\tilde{C}_d^{1/(2d)}$, so $R_2 \lesssim_d \exp(-c'_d n^{t/(4d)})$ for all such t and n, where $c'_d > 0$ depends only on d. But since

$$\int_{8d}^\infty \exp(-c'_d n^{t/(4d)})\,dt = \frac{4d}{\log n}\int_{n^2}^\infty s^{-1}\,e^{-c'_d s}\,ds \lesssim_d e^{-c'_d n^2}, \tag{2.6.10}$$

it follows from (2.6.7), (2.6.8), (2.6.9) and (2.6.10) that there exists $n'_d > 0$ depending only on d such that

$$\int_{8d}^{\infty} \mathbb{P}\biggl(\sup_{x\in\mathbb{R}^d} \log \hat{f}_n(x) > \frac{t}{2}\log n\biggr)\,dt \lesssim_d n^{-n/2} \tag{2.6.11}$$

for all $n \geq n'_d$. We deduce that

$$\mathbb{E}\biggl\{\sup_{x\in\mathbb{R}^d} \log \hat{f}_n(x)\biggr\} \leq \frac{\log n}{2}\biggl\{8d + \int_{8d}^{\infty} \mathbb{P}\biggl(\sup_{x\in C_n} \log \hat{f}_n(x) \geq \frac{t}{2}\log n\biggr)\,dt\biggr\} \lesssim_d \log n \tag{2.6.12}$$

for all $n \geq n'_d$. By increasing the multiplicative constants to deal with smaller values of n if necessary, we can ensure that (2.6.11) and (2.6.12) hold for all $n \geq d+1$.

Next, we address the second term on the left hand side of (2.6.1). Let $X \equiv (X^1,\ldots,X^d) \sim f_0$, and for $j = 1,\ldots,d$, let $f_{j|1:(j-1)}(\cdot\,|\,x^1,\ldots,x^{j-1})$ denote the conditional density of X^j given $(X^1,\ldots,X^{j-1}) = (x^1,\ldots,x^{j-1})$, where we adopt the convention that the $j=1$ case refers to the marginal density of X^1. By Cule et al. (2010, Proposition 1(a)), each of these densities is then log-concave. For $j = 1,\ldots,d$, let $F_{j|1:(j-1)}(\cdot\,|\,x^1,\ldots,x^{j-1})$ denote the corresponding distribution function, and define $U^j := F_{j|1:(j-1)}(X^j\,|\,X^1,\ldots,X^{j-1})$. Then $U^j\,|\,(X^1,\ldots,X^{j-1}) \sim U(0,1)$ for all j, so in particular each U^j has a marginal $U(0,1)$ distribution. In addition, for $j = 1,\ldots,d$, let

$$I_{j|1:(j-1)}(\cdot\,|\,X^1,\ldots,X^{j-1}) := f_{j|1:(j-1)}\bigl(F^{-1}_{j|1:(j-1)}(\cdot\,|\,X^1,\ldots,X^{j-1})\,|\,X^1,\ldots,X^{j-1}\bigr),$$

which by Bobkov (1996, Proposition A.1(c)) is positive and concave on $(0,1)$. We now need to understand how the functions $I_{j|1:(j-1)}$ transform under affine maps. To this end, consider a real-valued random variable Y with density f and distribution function F, and let $I := f \circ F^{-1}$. Now for $\mu \in \mathbb{R}$ and $\sigma > 0$, let $Z := \sigma Y + \mu$ and let $f_{\mu,\sigma}$, $F_{\mu,\sigma}$ and $I_{\mu,\sigma}$ denote the corresponding functions for Z. Then

$$f_{\mu,\sigma}(z) = \frac{1}{\sigma} f\biggl(\frac{z-\mu}{\sigma}\biggr), \quad F_{\mu,\sigma}(z) = F\biggl(\frac{z-\mu}{\sigma}\biggr), \quad F^{-1}_{\mu,\sigma}(u) = \sigma F^{-1}(u) + \mu,$$

so that

$$I_{\mu,\sigma}(u) = f_{\mu,\sigma}\bigl(F^{-1}_{\mu,\sigma}(u)\bigr) = \frac{1}{\sigma} f\bigl(F^{-1}(u)\bigr).$$

It follows from this and Lemma 3 in the online supplement to Kim et al. (2018) that there exists a universal constant $\alpha > 0$ such that for every $u \in (0,1)$ and $j \in \{1,\ldots,d\}$, we have

$$I_{j|1:(j-1)}(u\,|\,X^1,\ldots,X^{j-1}) \geq \frac{\alpha}{\mathrm{Var}^{1/2}(X^j\,|\,X^1,\ldots,X^{j-1})}\min(u, 1-u).$$

Therefore, if $X \sim f_0$, then for all $t > 0$, we have

$$\begin{aligned}
\mathbb{P}\biggl(\log\frac{1}{f_0(X)} \geq t\biggr) &= \mathbb{P}\bigl(f_0(X) \leq e^{-t}\bigr) = \mathbb{P}\Bigl(\textstyle\prod_{j=1}^d f_{j|1:(j-1)}(X^j\,|\,X^1,\ldots,X^{j-1}) \leq e^{-t}\Bigr) \\
&= \mathbb{P}\Bigl(\textstyle\prod_{j=1}^d I_{j|1:(j-1)}(U^j\,|\,X^1,\ldots,X^{j-1}) \leq e^{-t}\Bigr) \\
&\leq \mathbb{P}\Bigl(\min_{j=1,\ldots,d} I_{j|1:(j-1)}(U^j\,|\,X^1,\ldots,X^{j-1}) \leq e^{-t/d}\Bigr) \\
&\leq \mathbb{P}\biggl(\min_{j=1,\ldots,d} \frac{\alpha}{\mathrm{Var}^{1/2}(X^j\,|\,X^1,\ldots,X^{j-1})}\min(U^j, 1-U^j) \leq e^{-t/d}\biggr).
\end{aligned}$$

Also, the function $h(x) := e \vee \exp(\sqrt{x}/2)$ is convex and increasing on $[0,\infty)$. By applying Proposition 2.6.3(iii) to the density of X^j, which lies in $\mathcal{F}_1^{0,I}$, we find that

$$\begin{aligned}\mathbb{E}\bigl\{e^{\mathrm{Var}^{1/2}(X^j \,|\, X^1,\ldots,X^{j-1})/2}\bigr\} &\leq \mathbb{E}\bigl\{e^{\mathbb{E}^{1/2}((X^j)^2 \,|\, X^1,\ldots,X^{j-1})/2}\bigr\} \\ &\leq \mathbb{E}\bigl\{h\bigl(\mathbb{E}\{(X^j)^2 \,|\, X^1,\ldots,X^{j-1}\}\bigr)\bigr\} \\ &\leq \mathbb{E}\bigl\{e \vee \exp\left(|X^j|/2\right)\bigr\} \leq e + 2\int_0^\infty e^{-x/2+1}\,dx = 5e,\end{aligned}$$

where we have used Jensen's inequality to obtain the penultimate bound. Defining the event $B := \bigl\{\max_{j=1,\ldots,d} \mathrm{Var}^{1/2}(X^j \,|\, X^1,\ldots,X^{j-1}) \leq t\bigr\}$, we deduce that if $n \geq d+1$ and $X_1,\ldots,X_n \overset{\mathrm{iid}}{\sim} f_0$, then

$$\begin{aligned}&\mathbb{P}\left(\min_{j=1,\ldots,d} \frac{\alpha}{\mathrm{Var}^{1/2}(X^j \,|\, X^1,\ldots,X^{j-1})} \min(U^j, 1-U^j) \leq e^{-t/d}\right) \\ &\leq \mathbb{P}\left(\left\{\min_{j=1,\ldots,d} \frac{\alpha \min(U^j,1-U^j)}{\mathrm{Var}^{1/2}(X^j \,|\, X^1,\ldots,X^{j-1})} \leq e^{-t/d}\right\} \cap B\right) + \mathbb{P}(B^c) \\ &\leq 2\alpha^{-1} dte^{-t/d} + 5de^{1-t/2}.\end{aligned}$$

It follows that for all $t > 0$, we have

$$\mathbb{P}\left(\max_{i=1,\ldots,n} \log \frac{1}{f_0(X_i)} > \frac{t}{2}\log n\right) \leq n\,\mathbb{P}\left(\log\frac{1}{f_0(X)} > \frac{t}{2}\log n\right) \leq \frac{dt\log n}{\alpha n^{t/(2d)-1}} + \frac{5ed}{n^{t/4-1}}.$$

Since $\int_{8d}^\infty (t\log n)\, n^{1-t/(2d)}\,dt \lesssim_d n\int_{4\log n}^\infty (\log n)^{-1}\, se^{-s}\,ds \lesssim_d n^{-3}$, we conclude that

$$\int_{8d}^\infty \mathbb{P}\left(\max_{i=1,\ldots,n} \log\frac{1}{f_0(X_i)} > \frac{t}{2}\log n\right) dt \lesssim_d n^{-3} \tag{2.6.13}$$

and hence that

$$\mathbb{E}\left\{\max_{i=1,\ldots,n} \log\frac{1}{f_0(X_i)}\right\} \leq \frac{\log n}{2}\left\{8d + \int_{8d}^\infty \mathbb{P}\left(\max_{i=1,\ldots,n} \log\frac{1}{f_0(X_i)} > \frac{t}{2}\log n\right) dt\right\} \lesssim_d \log n \tag{2.6.14}$$

for all $n \geq d+1$. The required bounds (2.6.1) and (2.6.2) follow by combining (2.6.12) and (2.6.14), and (2.6.11) and (2.6.13) respectively. □

Recalling that $d_{\mathrm{H}}^2(\hat{f}_n, f_0) \leq \mathrm{KL}(\hat{f}_n, f_0) \leq d_X^2(\hat{f}_n, f_0)$, as mentioned in the introduction, we record here that in Kim and Samworth (2016, Theorem 5), the worst-case d_{H}^2 risk bounds for $\hat{f}_n$ in dimensions $d = 1,2,3$ can be strengthened to d_X^2 risk bounds of the same form. This requires only a small modification to the original proof, as we now explain.

Theorem 2.6.2. *Let $X_1,\ldots,X_n \overset{\mathrm{iid}}{\sim} f_0 \in \mathcal{F}_d$ with $n \geq d+1$, and let $\hat{f}_n$ denote the corresponding log-concave maximum likelihood estimator. Then*

$$\sup_{f_0 \in \mathcal{F}_d} \mathbb{E}\{d_X^2(\hat{f}_n, f_0)\} = \begin{cases} O(n^{-4/5}) & \text{if } d = 1 \\ O(n^{-2/3}\log n) & \text{if } d = 2 \\ O(n^{-1/2}\log n) & \text{if } d = 3. \end{cases} \tag{2.6.15}$$

Proof. In the original proof of Kim and Samworth (2016, Theorem 5), the key bracketing entropy bounds from Kim and Samworth (2016, Theorem 4) are converted into d_{H}^2 risk bounds by appealing to van de Geer (2000, Theorem 7.4), a result from empirical process theory that is restated as Theorem 5 in the online supplement to Kim and Samworth (2016). Note that

$d_X^2(\hat{f}_n, f_0) = n^{-1}\sum_{i=1}^n \log \frac{\hat{f}_n(X_i)}{f_0(X_i)} = \int \log(\hat{f}_n/f_0)\, d\mathbb{P}_n$, where $\mathbb{P}_n$ denotes the empirical measure of $X_1, \ldots, X_n$. In view of this, we can derive (2.6.15) from Kim and Samworth (2016, Theorem 4) by carrying out identical calculations to those in the proof of Kim and Samworth (2016, Theorem 5) but instead appealing to van de Geer (2000, Corollary 7.5). The latter is restated as Theorem 10 in the online supplement to Kim et al. (2018) and holds under the same conditions as those required for van de Geer (2000, Theorem 7.4). □

2.6.2 The envelope function for the class of isotropic log-concave densities on $\mathbb{R}$

In the proof of Lemma 2.6.1, we make use of Proposition 2.6.3, a result of independent interest that characterises the envelope function for the class $\mathcal{F}_1^{0,1} \equiv \mathcal{F}_1^{0,I}$ of all real-valued isotropic log-concave densities. Previously, it was known that $F(x) := \sup_{f \in \mathcal{F}_1^{0,1}} f(x) \leq 1$ for all $x \in \mathbb{R}$ (Lovász and Vempala, 2006, Lemma 5.5(a)) and that there exist $A > 0$ and $B \in \mathbb{R}$ such that $F(x) \leq e^{-A|x|+B}$ for all $x \in \mathbb{R}$ (e.g. Kim and Samworth, 2016, Theorem 2(a)). The proposition below shows that we can in fact take $A = B = 1$ and moreover that this is the optimal choice of A and B, in the sense that the bound above does not hold for all $x \in \mathbb{R}$ if either $A > 1$ or $A = 1$ and $B < 1$. Furthermore, there is a simple closed form expression for $F(x)$ when $|x| \leq 1$, and it is somewhat surprising that $F(x)$ increases as $|x|$ increases from 0 to 1.

Proposition 2.6.3. *The envelope function F for $\mathcal{F}_1^{0,1}$ is even and piecewise smooth, and has the following properties:*

(i) $F(x) = (2 - x^2)^{-1/2}$ *for all* $x \in (-1, 1)$;

(ii) $F(x) \geq e^{-(x+1)}$ *for all* $x \geq -1$ *and* $e^{x+1}F(x) \to 1$ *as* $x \to \infty$;

(iii) $F(x) \leq 1 \wedge e^{-|x|+1}$ *for all* $x \in \mathbb{R}$.

As a by-product of the proof, we obtain an explicit expression for F: see (2.6.27) below. Moreover, we will see that for each $x \in \mathbb{R}$, there exists a piecewise log-affine density f_x that achieves the supremum in the definition of $F(x)$. This extremal distribution f_x can take one of two forms depending on whether $|x| < 1$ or $|x| \geq 1$, and we treat these cases separately. The proof relies heavily on stochastic domination arguments based on the following lemma.

Lemma 2.6.4. *Let X, Y be real-valued random variables with densities f, g and corresponding distribution functions F, G respectively. Then we have the following:*

(i) If there exists $a \in \mathbb{R}$ such that $f \leq g$ on $(-\infty, a)$ and $f \geq g$ on (a, ∞), then $F \leq G$, i.e. X stochastically dominates Y. If in addition X and Y are integrable and f, g differ on a set of positive Lebesgue measure, then $\mathbb{E}(X) > \mathbb{E}(Y)$.

(ii) Suppose that there exist $a < b$ such that $f \geq g$ on (a, b) and $f \leq g$ on $(-\infty, a) \cup (b, \infty)$, and moreover that f and g are not equal almost everywhere when restricted to either $(-\infty, a)$ or (b, ∞). Then there exists a unique $c \in \mathbb{R}$ with $0 < F(c) = G(c) < 1$ such that $F \leq G$ on $(-\infty, c)$ and $F \geq G$ on (c, ∞). If in addition X and Y are square-integrable and $\mathbb{E}(X) = \mathbb{E}(Y)$, then $\mathrm{Var}(X) < \mathrm{Var}(Y)$.

Proof of Lemma 2.6.4. Note that $\mathbb{P}(X \geq t) = \int_t^\infty f(s)\, ds \geq \int_t^\infty g(s)\, ds = \mathbb{P}(Y \geq t)$ when $t \geq a$. Similarly, $\mathbb{P}(X \geq t) = 1 - \int_{-\infty}^t f(s)\, ds \geq 1 - \int_{-\infty}^t g(s)\, ds = \mathbb{P}(Y \geq t)$ when $t \leq a$. Part (i) now follows immediately from the identity

$$\mathbb{E}(X) = \mathbb{E}(X^+) - \mathbb{E}(X^-) = \int_0^\infty \bigl\{\mathbb{P}(X \geq s) - \mathbb{P}(X < -s)\bigr\}\, ds.$$

For (ii), $G - F$ is an (absolutely) continuous function that is increasing on the intervals $(-\infty, a)$ and (b, ∞), so the first assertion is an immediate consequence of the fact that $(G-F)(a) > 0 > (G-F)(b)$. Also, if W is a square-integrable random variable, then Fubini's theorem implies that

$$\int_0^\infty \int_s^\infty \mathbb{P}(W \geq t)\,dt\,ds = \mathbb{E}\biggl(\int_0^\infty \int_0^\infty \mathbb{1}_{\{W \geq t \geq s\}}\,dt\,ds\biggr) = \mathbb{E}\biggl(\int_0^\infty (W-s)\mathbb{1}_{\{W \geq s\}}\,ds\biggr). \quad (2.6.16)$$

Now since $\mathbb{E}\bigl(W \int_0^\infty \mathbb{1}_{\{W \geq s\}}\,ds\bigr) = \mathbb{E}\{(W^+)^2\}$ and

$$\mathbb{E}\biggl(\int_0^\infty s\,\mathbb{1}_{\{W \geq s\}}\,ds\biggr) = \int_0^\infty s\,\mathbb{P}(W \geq s)\,ds = \frac{1}{2}\int_0^\infty \mathbb{P}\bigl\{(W^+)^2 \geq s\bigr\}\,ds = \frac{1}{2}\,\mathbb{E}\{(W^+)^2\},$$

the right hand side of (2.6.16) is equal to $2^{-1}\,\mathbb{E}\{(W^+)^2\}$. By applying similar reasoning to W^-, we conclude that

$$\mathbb{E}(W^2) = \mathbb{E}\{(W^+)^2\} + \mathbb{E}\{(W^-)^2\} = 2\biggl(\int_0^\infty \int_s^\infty \bigl\{\mathbb{P}(W \geq t) + \mathbb{P}(W \leq -t)\bigr\}\,dt\,ds\biggr).$$

Since $\mathbb{P}(X \geq c+t) \leq \mathbb{P}(Y \geq c+t)$ and $\mathbb{P}(X \leq c-t) \leq \mathbb{P}(Y \leq c-t)$ for all $t \geq 0$, and since F and G do not agree almost everywhere by hypothesis, it follows from this that $\mathbb{E}\{(X-c)^2\} < \mathbb{E}\{(Y-c)^2\}$. This implies the second assertion in view of our assumption that $\mathbb{E}(X) = \mathbb{E}(Y)$. □

The proofs of parts (ii) and (iii) of Proposition 2.6.3 require some additional probabilistic input. For $K \in (0, \infty]$ and a non-degenerate random variable W that takes non-negative values, let W_K be a random variable whose distribution is that of W conditioned to lie in $[0, K)$. Letting Y be a random variable with an Exp(1) distribution, we now set

$$h(K) := \mathbb{E}(Y_K) = \frac{1-(K+1)\,e^{-K}}{1-e^{-K}} \quad (2.6.17)$$

$$V(K) := \mathrm{Var}(Y_K) = 1 - \frac{K^2}{2\,(\cosh K - 1)}. \quad (2.6.18)$$

It is easily verified that V is positive, strictly increasing and tends to 1 as $K \to \infty$. Also, h and V are smooth, so in particular, V has a smooth inverse $V^{-1}\colon (0,1) \to (0,\infty)$. Moreover, for each $\lambda \in (0,1]$, let W^λ be a random variable distributed as $\mathrm{Exp}(\lambda)$. We now make crucial use of the scaling property $W^\lambda \overset{d}{=} Y/\lambda$ of exponential random variables, a consequence of which is that we need only work with the functions h and V. Indeed, we have $\mathbb{E}(W_K^\lambda) = h(\lambda K)/\lambda$ and $\mathrm{Var}(W_K^\lambda) = V(\lambda K)/\lambda^2$, so we can find a unique

$$K = K(\lambda) := V^{-1}(\lambda^2)/\lambda \in (0,\infty) \quad (2.6.19)$$

such that $\mathrm{Var}(W_K^\lambda) = 1$. Thus, the density f_λ of $X_\lambda := W_{K(\lambda)}^\lambda - \mathbb{E}(W_{K(\lambda)}^\lambda)$ lies in $\mathcal{F}_1^{0,1}$ and is log-affine on its support $[-m(\lambda), a(\lambda)]$, where

$$m(\lambda) := \mathbb{E}(W_{K(\lambda)}^\lambda) = \frac{1}{\lambda}\biggl(1 - \frac{\lambda K}{e^{\lambda K} - 1}\biggr), \quad (2.6.20)$$

$$a(\lambda) := K(\lambda) - m(\lambda) = \frac{1}{\lambda}\biggl(\frac{\lambda K e^{\lambda K}}{e^{\lambda K} - 1} - 1\biggr) \quad (2.6.21)$$

are smooth, non-negative functions of λ. We now show that:

Lemma 2.6.5. *The functions m, a, K are smooth bijections from $(0,1)$ to $(1,\sqrt{3})$, $(\sqrt{3},\infty)$ and $(2\sqrt{3},\infty)$ respectively. Moreover, m is strictly decreasing and a, K are strictly increasing. We also have $(1-\lambda)K(\lambda) \to 0$ as $\lambda \nearrow 1$.*

While much of the following argument relies only on elementary analysis, a little probabilistic reasoning based on Lemma 2.6.4 helps to simplify the proof.

Proof of Lemma 2.6.5. The functions K, m and a defined in (2.6.19), (2.6.20) and (2.6.21) are certainly smooth, and since $V^{-1}(y) \to \infty$ as $y \nearrow 1$, we see that $m(\lambda) \to 1$ and $K(\lambda)$, $a(\lambda) \to \infty$ when $\lambda \nearrow 1$. Furthermore, $s := V^{-1}(\lambda^2) \to 0$ as $\lambda \to 0$, and since

$$V(s) = 1 - \frac{1}{1 + s^2/12 + o(s^2)} = \frac{s^2}{12} + o(s^2)$$

as $s \to 0$, we have $K(\lambda) = s\,V(s)^{-1/2} \to \sqrt{12} = 2\sqrt{3}$ as $\lambda \to 0$. Consequently, $m(\lambda) = K(\lambda)\bigl(1 - s/(e^s - 1)\bigr)/s \to 2\sqrt{3} \times 1/2 = \sqrt{3}$ as $\lambda \to 0$.

Finally, to show that $K(\lambda)(1-\lambda) \to 0$ as $\lambda \to \infty$, note that $\cosh y\,/e^y \to 1/2$ as $y \to \infty$ and moreover that for each $\delta > 0$, we have $y^2 e^{-y} < e^{-(1-\delta)y}$ for all sufficiently large y. This then implies that $V(y) > 1 - \exp(-y/2)$ for all sufficiently large y. Thus, $V^{-1}(\lambda^2) < 2\log(1-\lambda^2)$ for all λ sufficiently close to 1, so $K(\lambda)(1-\lambda) = V^{-1}(\lambda^2)(1-\lambda)/\lambda \to 0$ as $\lambda \nearrow 1$, as required.

It remains to show that m and a are strictly monotone. Fix $0 < \lambda_1 < \lambda_2 < 1$ and for $i = 1, 2$, let $\phi_{\lambda_i} := \log f_{\lambda_i}$ and recall that the density $f_{\lambda_i} \in \mathcal{F}_1^{0,1}$ is supported on $[-m(\lambda_i), a(\lambda_i)]$. In addition, observe that an (infinite) straight line in $\mathbb{R}^2$ with slope $-\lambda_2$ intersects the graph of ϕ_{λ_1} in exactly two points in $\mathbb{R}^2$, one of which has x-coordinate $a(\lambda_1)$. Now if the graphs of $\phi_{\lambda_1}, \phi_{\lambda_2}$ intersect in at most two points, then the densities $f_{\lambda_1}, f_{\lambda_2} \in \mathcal{F}_1^{0,1}$ satisfy one of the two sets of hypotheses in Lemma 2.6.4. However this then implies that either the means or the variances of $f_{\lambda_1}, f_{\lambda_2}$ do not match, which yields a contradiction. Therefore, it follows that $m(\lambda_2) < m(\lambda_1)$ and $a(\lambda_2) > a(\lambda_1)$.

The fact that K is strictly increasing follows readily from the observation that the function $s \mapsto s^{-2} - 2^{-1}(\cosh s - 1)^{-1}$ is strictly decreasing on $(0, \infty)$, as can be seen by applying the simple fact Lemma 2.6.6 below. $\square$

Lemma 2.6.6. *If $\sum_{n\geq 0} a_n z^n$ and $\sum_{n \geq 0} b_n z^n$ are power series with infinite radii of convergence such that $a_n, b_n > 0$ for all $n \geq 0$ and $(a_n/b_n)_{n\geq 0}$ is a strictly decreasing sequence, then $z \mapsto \bigl(\sum a_n z^n\bigr)/\bigl(\sum b_n z^n\bigr)$ is a strictly decreasing function of $z \in (0,\infty)$.*

Proof. Fix $0 < w < z$ and let $c_n := a_n/b_n$ for each n. Then for fixed $n > m \geq 0$, we have $c_n < c_m$, which implies that $c_n z^n w^m + c_m z^m w^n < c_n z^m w^n + c_m z^n w^m$. Thus, summing over all $m, n \geq 0$, we obtain the desired conclusion that

$$\begin{aligned}\bigl(\textstyle\sum_{n\geq 0} a_n z^n\bigr)\bigl(\sum_{m\geq 0} b_m w^m\bigr) &= \textstyle\sum_{n,m\geq 0} c_n b_n b_m z^n w^m \\ &< \textstyle\sum_{n,m\geq 0} c_n b_n b_m z^m w^n = \bigl(\sum_{n\geq 0} a_n w^n\bigr)\bigl(\sum_{m\geq 0} b_m z^m\bigr).\end{aligned}$$ $\square$

Proof of Proposition 2.6.3. For a fixed $x \in (-1, 1)$, we make the ansatz

$$f_x(w) := C\left\{\exp\left(-\frac{w-x}{a_1}\right)\mathbb{1}_{\{w\geq x\}} + \exp\left(\frac{w-x}{a_2}\right)\mathbb{1}_{\{w<x\}}\right\}, \tag{2.6.22}$$

where $C, a_1, a_2 > 0$ are to be determined. Note that $\log f_x$ is continuous on $\mathbb{R}$ and affine on the intervals $(-\infty, x]$ and $[x, \infty)$. If we are to ensure that $f_x \in \mathcal{F}_1^{0,1}$, then the parameters $C, a_1, a_2 > 0$ must satisfy the constraints

$$C(a_1 + a_2) = 1 \tag{2.6.23}$$

$$C(a_2^2 - a_1^2) = x \tag{2.6.24}$$

$$C\bigl\{2(a_1^3 + a_2^3) + 2x(a_1^2 - a_2^2) + x^2(a_1 + a_2)\bigr\} = 1, \tag{2.6.25}$$

which respectively guarantee that f_x integrates to 1 and has mean 0 and variance 1. The first two equations yield $a_1 = (C^{-1} - x)/2$ and $a_2 = (C^{-1} + x)/2$, so in particular we require $Cx < 1$. After substituting these expressions into the final equation, we conclude that $1 + x^2 = 2C(a_1^3 + a_2^3) = 2x^2 + (C^{-2} - x^2)/2$, so $C = (2 - x^2)^{-1/2}$. Since $|x| < 1$, it is indeed the case that $Cx < 1$, so these equations uniquely determine the form of f_x in terms of x.

Next, to show that $g(x) \leq C = f_x(x)$ for all $g \in \mathcal{F}_1^{0,1}$, we work on the logarithmic scale and suppose for a contradiction that there exists $g \in \mathcal{F}_1^{0,1}$ such that $g(x) > C$. Now since the functions $\phi := \log g$ and $\phi_x := \log f_x$ are concave and upper semi-continuous, it follows from the assumption $\phi(x) > \phi_x(x)$ that the graphs of ϕ and ϕ_x (viewed as subsets of $\mathbb{R}^2$) intersect in at most one point in each of the regions $(-\infty, x) \times \mathbb{R}$ and $(x, \infty) \times \mathbb{R}$. Note that here, we also take into account those x' which satisfy $\phi(x') \geq \phi_x(x')$ and which correspond to intersection points on the boundary of the support of g. To obtain the required contradiction, observe that the densities $g, f_x \in \mathcal{F}_1^{0,1}$ must therefore satisfy one of the two sets of hypotheses in Lemma 2.6.4. It follows from this that either the means or the variances of g, f_x do not match. This concludes the proof of part (i) of the proposition.

If instead our fixed $x \in \mathbb{R}$ satisfies $|x| \geq 1$, then the previous system of equations does not admit suitable solutions, so we take a different approach. Suppose first that there exists a compactly supported density in $\mathcal{F}_1^{0,1}$ of the form

$$f_x(w) := C \exp\{-\lambda(w - x)\} \mathbb{1}_{\{w \in [-a, x]\}}, \tag{2.6.26}$$

for some $C > 0$, $a \in (0, \infty]$ and $\lambda \in \mathbb{R}$. Then by appealing to Lemma 2.6.4 and arguing as in the previous paragraph, it follows that $F(x) = f_x(x)$; the key observation is that if there did exist $g \in \mathcal{F}_1^{0,1}$ satisfying $g(x) > f_x(x)$, then the graphs of g and f_x would intersect in either one or two points (in the sense described above), and these would necessarily lie in the region $[-a, x) \times \mathbb{R}$.

It therefore remains to show that, for each $x \in \mathbb{R}$ with $|x| \geq 1$, the class $\mathcal{F}_1^{0,1}$ does indeed contain a log-affine density f_x of this type (which in view of Lemma 2.6.4 is clearly unique if it exists). To see this, we reparametrise the densities of the form (2.6.26) in terms of λ, and then appeal to (2.6.20), (2.6.21), Lemma 2.6.5 and the probabilistic setup on which these are based. When $x \in (1, \sqrt{3})$, we can take f_x to be the density of $-X_\lambda$ with $\lambda = m^{-1}(x)$, and when $x \in (\sqrt{3}, \infty)$, we can take f_x to be the density of X_λ with $\lambda = a^{-1}(x)$. We can then argue by symmetry to handle negative values of x.

Finally, we consider the borderline cases $|x| = 1, \sqrt{3}$. If $|x| = 1$, then the extremal density f_x is the density of $\pm(Y - 1)$ where $Y \sim \mathrm{Exp}(1)$: this can be realised either as the limit of (2.6.22) as $|x| \nearrow 1$ or as the limit of (2.6.26) as $|x| \searrow 1$, so (unsurprisingly) F is continuous at 1. The case $|x| = \sqrt{3}$ corresponds to $\lambda = 0$; indeed, f_x is the density of $U[-\sqrt{3}, \sqrt{3}]$ in this instance.

In summary, using the fact that f_x integrates to 1 for each x, we deduce that

$$F(x) = f_x(x) = \begin{cases} \lambda\bigl(e^{\lambda K(\lambda)} - 1\bigr)^{-1} & \text{with } \lambda = a^{-1}(|x|) \text{ when } |x| > \sqrt{3} \\ (2\sqrt{3})^{-1} & \text{when } |x| = \sqrt{3} \\ \lambda\bigl(1 - e^{-\lambda K(\lambda)}\bigr)^{-1} & \text{with } \lambda = m^{-1}(|x|) \text{ when } 1 < |x| < \sqrt{3} \\ (2 - x^2)^{-1/2} & \text{when } |x| \leq 1, \end{cases} \tag{2.6.27}$$

which is smooth on $(-1, 1)$ and $(-\infty, -1) \cup (1, \infty)$. Also, $a \circ m^{-1}$ is a smooth and strictly decreasing function from $(1, \sqrt{3})$ to $(\sqrt{3}, \infty)$, and the values of F on these intervals are related by the identity

$$F(a(\lambda)) = F(m(\lambda)) e^{-\lambda K(\lambda)}, \tag{2.6.28}$$

which holds for all $\lambda \in (0,1)$. We now return to the assertions in part (ii) of the proposition. The first of these follows immediately from the fact that the density of an $\mathrm{Exp}(1)-1$ random variable lies in $\mathcal{F}_1^{0,1}$. For the second, we write $\lambda = a^{-1}(|x|)$, and in view of (2.6.27), it suffices to compute the ratio of $\lambda/(e^{\lambda K(\lambda)}-1)$ and $e^{-a(\lambda)-1} = e^{-K(\lambda)+m(\lambda)-1}$ as $\lambda \nearrow 1$. Note that $\log\lambda \to 0$ and $m(\lambda) \to 1$ as $\lambda \nearrow 1$. Thus, after taking logarithms, it is enough to consider the difference of $\lambda K(\lambda)$ and $K(\lambda)$, which does indeed tend to 0 by the final part of Lemma 2.6.5. This completes the proof of (ii), and also shows that there exists a constant $B \in \mathbb{R}$ such that $F(x) \le \exp(-|x|+B)$ for all $x \in \mathbb{R}$.

To establish part (iii) of the result, it remains to show that we can take $B = 1$. The expressions above can be made more analytically tractable by reparametrising everything in terms of $s = V^{-1}(\lambda^2) = \lambda K(\lambda)$, which is strictly increasing in $\lambda \in (0,1)$, so in a slight abuse of notation, we start by redefining

$$\begin{aligned} V(s) &= 1 - 2^{-1}s^2/(\cosh s - 1), \\ K(s) &= s\,V(s)^{-1/2}, \\ m(s) &= \bigl(1 - s/(e^s-1)\bigr)\,V(s)^{-1/2}, \\ a(s) &= \bigl(-1 + se^s/(e^s-1)\bigr)\,V(s)^{-1/2} \end{aligned}$$

as functions of $s \in (0,\infty)$. Lemma 2.6.5 implies that all of these are strictly monotone. In view of (2.6.27), we need to show that

$$V(s)^{1/2}\,e^{m(s)-1}\,(1-e^{-s})^{-1} \le 1; \tag{2.6.29}$$

$$V(s)^{1/2}\,e^{a(s)-1}\,(e^{s}-1)^{-1} \le 1 \tag{2.6.30}$$

for all $s \in (0,\infty)$. First we address (2.6.29), which corresponds to values of $x \in (1,\sqrt{3})$. This can be verified directly by numerical calculation for $s \in (0,5]$. Indeed, for $s \in (0,3/2]$, the left hand side can be rewritten as

$$K(s)^{-1}\,e^{m(s)-1}\,\frac{s}{1-e^{-s}}.$$

For $s \in (0,1]$, this is bounded above by $(2\sqrt{3})^{-1}\,e^{\sqrt{3}-1}\,s/(1-e^{-s}) \le 1$ in view of Lemma 2.6.5, and for $s \in [1,3/2]$, this is at most $K(1)^{-1}\,e^{m(1)-1}\,s/(1-e^{-s}) \le 1$. Similarly, for each $k \in \{3,\ldots,9\}$, the left hand side of (2.6.29) is at most

$$V\left(\frac{k+1}{2}\right)^{1/2} e^{m(k/2)-1}\,(1-e^{-k/2})^{-1}$$

for all $s \in [k/2,(k+1)/2]$, and all these values can be checked to be less than 1, as required.

Now we present a general argument that handles the case $s \ge 5$. We certainly have

$$1 - s^2(e^s-2)^{-1} \le V(s) \le 1 - s^2(e^s-1)^{-1}$$

for all $s \ge 0$, and we claim that

$$1 - s^2e^{-s}/2 \ge \sqrt{V(s)} \ge \left(1 - \frac{s^2}{e^s-2}\right)^{1/2} \ge 1 - s^2e^{-s}/2 - s^4e^{-2s}/2 \tag{2.6.31}$$

for all $s \ge 5/2$. To obtain the final inequality, observe that $(1-z)^{1/2} \ge 1 - z/2 - z^2/4$ for all $0 \le z \le 2(\sqrt{2}-1)$ and that $u := s^2(e^s-2)^{-1} \le 2^2/(e^2-2) < 2(\sqrt{2}-1)$ for $s \ge 2$, so it is enough to prove that the right hand side above is at most $1 - u/2 - u^2/4$. This reduces to showing that $s^2(1-2e^{-s}) - s^2(e^{-s} + (e^s-2)^{-1}) - 2 \ge 0$ for all $s \ge 5/2$, but as the left hand side of this final inequality is an increasing function of s which is non-negative at $s = 5/2$, the claim in (2.6.31) follows.

The original inequality (2.6.29) can be rewritten in the form

$$\frac{1}{\sqrt{V(s)}}\left(1 - \frac{s}{e^s - 1}\right) - 1 \leq \log\left(\frac{1 - e^{-s}}{\sqrt{V(s)}}\right),$$

and since $s^2 \leq e^s$ when $s \geq 0$, we have $e^{-s}(s^2/2 - 1)(1 - s^2e^{-s}/2)^{-1} \leq 1$. So by the bounds in (2.6.31) and the fact that $\log(1 + z) \geq z - z^2/2$ for $|z| < 1$, it is enough to show that

$$\frac{1 - se^{-s}}{1 - s^2e^{-s}/2 - s^4e^{-2s}/2} - 1 \leq e^{-s}\frac{s^2/2 - 1}{1 - s^2e^{-s}/2}\left(1 - \frac{e^{-s}(s^2/2 - 1)}{2\,(1 - s^2e^{-s}/2)}\right).$$

This is equivalent to showing that

$$\frac{(s^2 - 2s) + s^4e^{-s}}{s^2 - 2} \leq \left(1 - \frac{s^4e^{-2s}}{2\,(1 - s^2e^{-s}/2)}\right)\left(1 - \frac{e^{-s}(s^2/2 - 1)}{2\,(1 - s^2e^{-s}/2)}\right)$$

for all $s \geq 5$. In fact, we will establish the slightly stronger bound

$$\frac{(s^2 - 2s) + s^4e^{-s}}{s^2 - 2} \leq 1 - \frac{s^4e^{-2s} + e^{-s}(s^2/2 - 1)}{2\,(1 - s^2e^{-s}/2)}$$

for all $s \geq 5$. After clearing denominators and simplifying, we arrive at the equivalent inequality

$$4e^s(s - 1) + 2s^4e^{-s} + 4s^2 \geq 5s^4/2 + 2s^3 + 2,$$

which certainly holds whenever $s \geq 5$. Indeed, $16e^s - 5s^4/2 - 2s^3 \geq 0$ for all $s \geq 0$, since $5s^4e^{-s} + 4s^3e^{-s} \leq 5(4/e)^4 + 4(3/e)^3 \leq 32$, so we are done.

Now that we have established (2.6.29), it is relatively straightforward to obtain (2.6.30). For $s \leq 3$, we again proceed by direct calculation: here, the left hand side equals

$$K(s)^{-1}\,e^{a(s)-1}\,l(s),$$

where $l(s) := s/(e^s - 1)$ for $s > 0$ and $l(0) = 1$. Each of the terms in this product is a monotone in s by Lemma 2.6.5, so for each $k = 0, 1, 2$ and for all $s \in [k, k+1]$, their product is at most $(2\sqrt{3})^{-1}\,e^{a(k+1)-1}\,l(k) \leq 1$. On the other hand, for $s \geq 3$, the desired result will follow if we can establish that $a(s) \leq m(s) + s$. This is equivalent to the inequality

$$\sqrt{V(s)} \geq 1 - 2/s + 2/(e^s - 1), \tag{2.6.32}$$

so it suffices to prove that the lower bound in (2.6.31) is at least $1 - 2/s + 2/(e^s - 1)$, which amounts to showing that

$$s^3e^{-s}/2 + s^5e^{-2s}/2 + 2s\,(e^s - 1)^{-1} \leq 2$$

for all $s \geq 3$. To establish this, we simply bound each summand on the left hand side by its global maximum in $[3, \infty)$. This completes the proof of (iii). □

2.6.3 Local bracketing entropy bounds

The aim of this section is to prove some local bracketing entropy results that form the backbone of the proofs of Theorems 2.2.3 and 2.3.1 in Sections 2.2 and 2.3 respectively. Theorem 2.2.3 is a consequence of the key local bracketing entropy bound stated as Proposition 2.5.1 in Section 2.5.1, which in turn builds on two intermediate results that we establish below, namely Propositions 2.6.8 and 2.6.9. By modifying the proofs of these two results, we obtain the analogous bounds in Propositions 2.6.10 and 2.6.11, which constitute the crux of the proof of Theorem 2.3.1. Throughout, we rely heavily on the technical tools developed in Section 2.7.2. We will use the notation introduced at the start of Sections 2.1.1, 2.5 and 2.7, as well as the key definitions from Sections 2.2 and 2.3.

We start by collecting together some global bracketing entropy bounds which are minor modifications of those that appear in Gao and Wellner (2017), Kim and Samworth (2016), and Kim et al. (2018). Recall that, as in Kim and Samworth (2016), we define $h_2, h_3 \colon (0,\infty) \to (0,\infty)$ by $h_2(x) := x^{-1}\log_+^{3/2}(x^{-1})$ and $h_3(x) := x^{-2}$ respectively. For measurable $f, g \colon \mathbb{R}^d \to \mathbb{R}$, let $L_2(f,g) := \bigl\{\int_{\mathbb{R}^d}(f-g)^2\bigr\}^{1/2}$. In addition, denote by $\mathcal{K}^b \equiv \mathcal{K}_d^b$ the collection of all compact, convex sets $K \subseteq \mathbb{R}^d$ with non-empty interior. For $K \in \mathcal{K}^b$, let $\Phi(K) := \{\phi|_K : \phi \in \Phi\}$, and for $-\infty \leq B_1 < B_2 < \infty$ and $K_1,\ldots,K_m \in \mathcal{K}^b$, define $\Phi_{B_1,B_2}(K_1,\ldots,K_m) := \{\phi \colon \bigcup_{j=1}^m K_j \to [B_1,B_2] : \phi|_{K_j} \in \Phi(K_j) \text{ for all } 1 \leq j \leq m\}$ and $\mathcal{G}_{B_1,B_2}(K_1,\ldots,K_m) := \bigl\{e^{\phi}\,\mathbb{1}_{\bigcup_{j=1}^m K_j} : \phi \in \Phi,\ \phi|_{\bigcup_{j=1}^m K_j} \in \Phi_{B_1,B_2}(K_1,\ldots,K_m)\bigr\}$.

Proposition 2.6.7. *For $d \in \mathbb{N}$, let $S_1,\ldots,S_m \subseteq \mathbb{R}^d$ be d-simplices with pairwise disjoint interiors. If $\varepsilon > 0$ and $-\infty < B_1 < B_2 < \infty$, then*

$$H_{[\,]}\bigl(\varepsilon, \mathcal{G}_{B_1,B_2}(S_1,\ldots,S_m), d_{\mathrm{H}}\bigr) \lesssim_d m\left(\frac{e^{B_2/2}\,(B_2-B_1)\,\mu_d^{1/2}\bigl(\bigcup_{j=1}^m S_j\bigr)}{\varepsilon}\right)^{d/2}. \tag{2.6.33}$$

Suppose henceforth that $d \in \{2,3\}$. If $K \in \mathcal{K}^b \equiv \mathcal{K}_d^b$ and $\varepsilon > 0$, then

$$H_{[\,]}\bigl(\varepsilon, \mathcal{G}_{B_1,B_2}(K), d_{\mathrm{H}}\bigr) \lesssim h_d\left(\frac{\varepsilon}{e^{B_2/2}\,(B_2-B_1)\,\mu_d^{1/2}(K)}\right) \tag{2.6.34}$$

whenever $-\infty < B_1 < B_2 < \infty$, and

$$H_{[\,]}\bigl(\varepsilon, \mathcal{G}_{-\infty,B}(K), d_{\mathrm{H}}\bigr) \lesssim h_d\left(\frac{\varepsilon}{e^{B/2}\mu_d^{1/2}(K)}\right) \tag{2.6.35}$$

for all $B \in \mathbb{R}$. Finally, for any family of sets $K_1,\ldots,K_m \in \mathcal{K}^b$ with pairwise disjoint interiors, we can obtain bounds for $H_{[\,]}\bigl(\varepsilon, \mathcal{G}_{B_1,B_2}(K_1,\ldots,K_m), d_{\mathrm{H}}\bigr)$ and $H_{[\,]}\bigl(\varepsilon, \mathcal{G}_{-\infty,B}(K_1,\ldots,K_m), d_{\mathrm{H}}\bigr)$ by multiplying the right hand sides of (2.6.34) and (2.6.35) respectively by m, and replacing $\mu_d(K)$ with $\mu_d\bigl(\bigcup_{j=1}^m K_j\bigr)$ throughout.

Proof. We first address (2.6.33), which is a d-dimensional version of Proposition 7 in the online supplement to Kim et al. (2018). First, for a fixed $\varepsilon > 0$, set $D := \bigcup_{j=1}^m S_j$ and $\varepsilon_j := \{\mu_d(S_j)/\mu_d(D)\}^{1/2}\,\varepsilon$ for each $1 \leq j \leq m$, and observe that by Gao and Wellner (2017, Theorem 1.1(ii)), we have

$$\begin{aligned} H_{[\,]}\bigl(\varepsilon, \Phi_{B_1,B_2}(S_1,\ldots,S_m), L_2\bigr) &\leq \sum_{j=1}^m H_{[\,]}\bigl(\varepsilon_j, \Phi_{B_1,B_2}(S_j), L_2\bigr) \lesssim_d \sum_{j=1}^m \left(\frac{(B_2-B_1)\,\mu_d^{1/2}(S_j)}{\varepsilon_j}\right)^{d/2} \\ &\lesssim_d m\left(\frac{(B_2-B_1)\,\mu_d^{1/2}(D)}{\varepsilon}\right)^{d/2}. \end{aligned} \tag{2.6.36}$$

To obtain (2.6.33), fix $\varepsilon > 0$ and set $\zeta := 2\varepsilon e^{-B_2/2}$. We deduce from (2.6.36) that there exists a bracketing set $\{[\phi_j^L, \phi_j^U] : 1 \leq j \leq M\}$ for $\Phi_{B_1,B_2}(S_1,\ldots,S_m)$ such that $L_2(\phi_j^L, \phi_j^U) \leq \zeta$ and $\phi_j^U \leq B_2$, where $\log M$ is bounded above by the right hand side of (2.6.33) up to a multiplicative factor that depends only on d. Since

$$\int_D \bigl(e^{\phi_j^U/2} - e^{\phi_j^L/2}\bigr)^2 \leq \frac{e^{B_2}}{4}\int_D \bigl(\phi_j^U - \phi_j^L\bigr)^2 \leq \varepsilon^2,$$

it follows that $\{[e^{\phi_j^L}, e^{\phi_j^U}] : 1 \leq j \leq M\}$ is an ε-Hellinger bracketing set for the class $\{f|_D : f \in \mathcal{G}_{B_1,B_2}(S_1,\ldots,S_m)\}$, as required.

In view of Proposition 4 in the online supplement to Kim and Samworth (2016), a similar proof to that given above yields (2.6.34). As for (2.6.35), we fix $d \in \{2,3\}$ and begin by outlining a simple scaling argument that allows us to deduce the general result from the special case where $B = -2$ and $\mu_d(K) = 1$. For $B' \in \mathbb{R}$ and $K' \in \mathcal{K}_d^b$, let $K := \lambda^{-1}K'$ and $\lambda := \mu_d(K')^{1/d}$, and suppose that we have already shown that

$$H_{[\,]}\bigl(\varepsilon, \mathcal{G}_{-\infty,-2}(K), d_{\mathrm{H}}\bigr) \lesssim h_d(\varepsilon) \tag{2.6.37}$$

for all $\varepsilon > 0$. Then for each $\varepsilon > 0$, we can find a bracketing set $\{[f_j^L, f_j^U] : 1 \leq j \leq M\}$ for $\mathcal{G}_{-\infty,-2}(K)$ such that

$$\int_K \Bigl(\sqrt{f_j^U} - \sqrt{f_j^L}\Bigr)^2 \leq \varepsilon^2 e^{-(B'+2)}\lambda^{-d}$$

for each $1 \leq j \leq M$ and $\log M \lesssim h_d\bigl(\varepsilon e^{-(B'+2)/2}\lambda^{-d/2}\bigr) \lesssim h_d\bigl(\varepsilon e^{-B'/2}\mu_d^{-1/2}(K')\bigr)$. Since every $g \in \mathcal{G}_{-\infty,B'}(K')$ takes the form $x \mapsto e^{B'+2}f(\lambda^{-1}x)$ for some $f \in \mathcal{G}_{-\infty,-2}(K)$, it follows that $\mathcal{G}_{-\infty,B'}(K')$ is covered by the brackets $\{[g_j^L, g_j^U] : 1 \leq j \leq M\}$ defined by

$$g_j^L(x) := e^{B'+2}f_j^L(\lambda^{-1}x), \quad g_j^U(x) := e^{B'+2}f_j^U(\lambda^{-1}x).$$

To see that this constitutes a valid ε-bracketing set and thereby implies the desired conclusion, observe that

$$\begin{aligned}\int_{K'} \Bigl(\sqrt{g_j^U} - \sqrt{g_j^L}\Bigr)^2 &= e^{B'+2}\int_{K'} \Bigl\{f_j^U(\lambda^{-1}x)^{1/2} - f_j^L(\lambda^{-1}x)^{1/2}\Bigr\}^2\,dx \\ &= e^{B'+2}\lambda^d \int_K \Bigl(\sqrt{f_j^U} - \sqrt{f_j^L}\Bigr)^2 \leq \varepsilon^2\end{aligned}$$

for all $1 \leq j \leq M$, as required. Therefore, it remains to establish (2.6.37). This will require only a few small adjustments to the arguments in steps 2 and 3 of the proof of Theorem 4 in Kim and Samworth (2016), where it was shown that

$$H_{[\,]}\bigl((4+e)\varepsilon, \mathcal{G}_{-\infty,-2}(K), d_{\mathrm{H}}\bigr) = H_{[\,]}\bigl((4+e)\varepsilon, \mathcal{G}_{-\infty,-1}(K), L_2\bigr) \lesssim h_d(\varepsilon) \tag{2.6.38}$$

for all $0 < \varepsilon < e^{-1}$ when $K = [0,1]^d$. For $\varepsilon > e^{-1}$, we may use a single bracketing pair $[f^L, f^U]$ with $f^L \equiv 0$ and $f^U \equiv 1$, so the left hand side is 0 in this case. Therefore (2.6.38) holds for all $\varepsilon > 0$ when $K = [0,1]^d$. Furthermore, since the bounds in Propositions 2 and 4 in the online supplement to Kim and Samworth (2016) depend on the convex domain K only through $\mu_d(K)$, all the intermediate steps in the proof of (2.6.38) in Kim and Samworth (2016) remain valid when $[0,1]^d$ is replaced with an arbitrary $K \in \mathcal{K}_d^b$ with $\mu_d(K) = 1$. This crucial observation completes the proof of (2.6.37) and hence that of (2.6.35).

The final assertion of Proposition 2.6.7 follows from (2.6.34) and (2.6.35) in much the same way that (2.6.33) follows from the special case $m = 1$. □

As a first step towards proving Proposition 2.5.1 for general $f_0 \in \mathcal{F}^1(\mathcal{P}^m)$, we consider here the special case where K is a d-simplex and $f_0 = f_K = \mu_d(K)^{-1}\mathbb{1}_K$ is the uniform density on K. For further discussion of the proof techniques we employ, see the discussion after the statement of

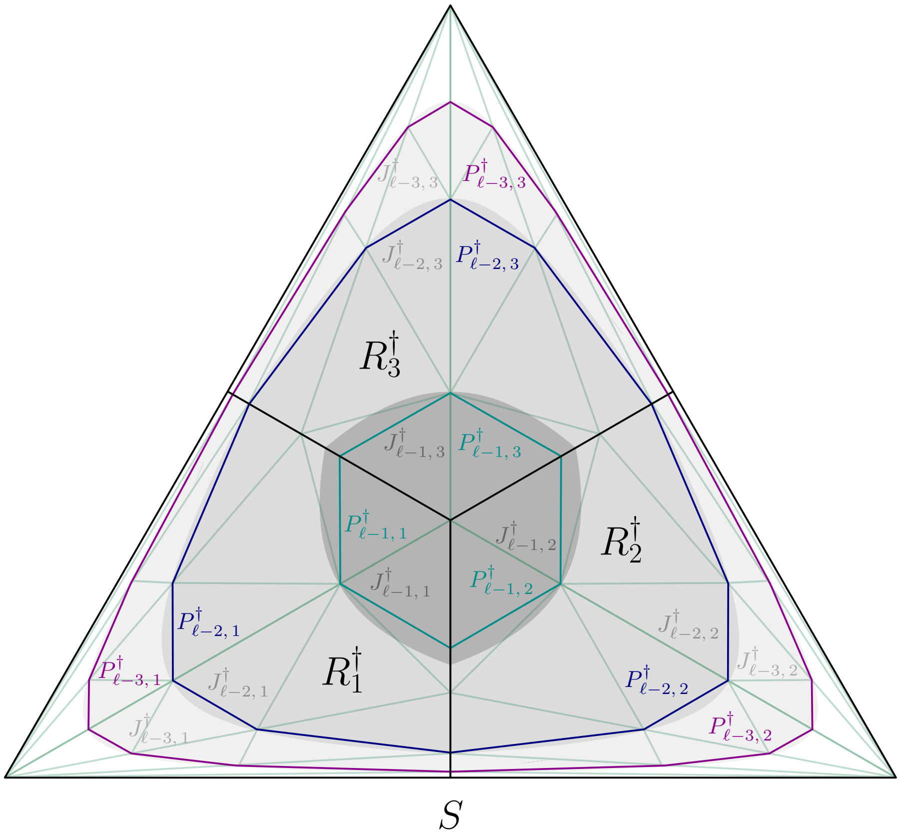

Figure 2.1: Illustration of the proof of Proposition 2.6.8 when $d = 2$ (and $\delta < 1/24$, so that $\ell \geq 4$). The polytopes $R_1^\dagger, R_2^\dagger, R_3^\dagger \subseteq S$ are demarcated by the black lines. For $i \in \{\ell-3, \ell-2, \ell-1\}$ and $j \in \{1, 2, 3\}$, the 'invelopes' $J_{i,j}^\dagger \subseteq R_j^\dagger$ are represented by the grey shaded regions (see Lemma 2.7.19) and the boundaries of the approximating polytopes $P_{i,j}^\dagger \subseteq J_{i,j}^\dagger$ are outlined in colour (see Corollary 2.7.22). Moreover, the regions between the nested polytopes $R_j^\dagger \supseteq P_{1,j}^\dagger \supseteq P_{2,j}^\dagger \supseteq \cdots \supseteq P_{\ell,j}^\dagger$ may be triangulated, as is indicated by the green line segments. The main reason for considering these sets is that by Lemma 2.7.19(iii), every $f \in \mathcal{G}(f_S, \delta)$ satisfies a pointwise lower bound $\log f + \log \mu_d(S) \geq -2^{-i+2}$ on $J_{i,j}^\dagger \supseteq P_{i,j}^\dagger$.

Theorem 2.2.3 in Section 2.2 and page 84 of Section 2.7.2. See Figure 2.1 for an illustration of the proof. For $d \in \mathbb{N}$, we define a 'canonical' regular d-simplex $\triangle \equiv \triangle_d := \mathrm{conv}\{e_1, \ldots, e_{d+1}\} \subseteq \mathbb{R}^{d+1}$ of side length $\sqrt{2}$, which will be viewed as a subset of its affine hull, namely $\mathrm{aff}\,\triangle = \{x = (x_1, \ldots, x_{d+1}) \in \mathbb{R}^{d+1} : \sum_{j=1}^{d+1} x_j = 1\}$.

Proposition 2.6.8. *Let $d \in \{2, 3\}$. If $0 < \varepsilon < \delta < (d+1)^{-d/2}$ and $S \subseteq \mathbb{R}^d$ is a d-simplex, then*

$$H_{[\,]}\big(2^{1/2}\varepsilon, \mathcal{G}(f_S, \delta), d_{\mathrm{H}}\big) \lesssim \left(\frac{\delta}{\varepsilon}\right) \log^{3/2}\left(\frac{1}{\delta}\right) \log^{3/2}\left(\frac{\log(1/\delta)}{\varepsilon}\right) =: H_2(\delta, \varepsilon) \tag{2.6.39}$$

when $d = 2$ and

$$H_{[\,]}\big(2^{1/2}\varepsilon, \mathcal{G}(f_S, \delta), d_{\mathrm{H}}\big) \lesssim \left(\frac{\delta}{\varepsilon}\right)^2 \log^4\left(\frac{1}{\delta}\right) + \left(\frac{\delta}{\varepsilon}\right)^{3/2} \log^{21/4}\left(\frac{1}{\delta}\right) =: H_3(\delta, \varepsilon) \tag{2.6.40}$$

when $d = 3$.

Proof. Fix $d \in \{2, 3\}$ and suppose that $0 < \varepsilon < \delta < (d+1)^{-d/2}$. In addition, define $\varepsilon' := \varepsilon/\sqrt{d+1}$ and $\ell := \lceil \log_2((d+1)^{-d/2}\delta^{-1}) \rceil$, so that ℓ is the smallest integer i such that $4^i\delta^2 \geq (d+1)^{-d}$, and note that $1 \leq \ell \lesssim \log(1/\delta)$. Since d_{H} is affine invariant, we may assume without loss of generality that S is a regular d-simplex with side length $\sqrt{2}$. Then since $\triangle \equiv \triangle_d = \mathrm{conv}\{e_1, \ldots, e_{d+1}\} \subseteq \mathbb{R}^{d+1}$ is also a d-simplex with side length $\sqrt{2}$, there is an (affine) isometry $T\colon \mathrm{aff}\,\triangle \to \mathbb{R}^d$ such that

$T(\triangle) = S$. For each $j \in \{1, \ldots, d+1\}$, define $R_j \subseteq \triangle$ as in (2.7.22) and let $R_j^\dagger := T(R_j) \subseteq S$. Then S is the union of the polytopes $R_1^\dagger, \ldots, R_{d+1}^\dagger$, whose interiors are pairwise disjoint.

Fix $j \in \{1, \ldots, d+1\}$, and for each $i \in \{1, \ldots, \ell-1\}$, define $J_{i,j}^\dagger := T\bigl(R_j \cap J_{4^i\delta^2}^\triangle\bigr)$ and $P_{i,j}^\dagger := T\bigl(P_{4^i\delta^2,\,j}^\triangle\bigr)$, where $J_{4^i\delta^2}^\triangle \subseteq \triangle$ and $P_{4^i\delta^2,\,j}^\triangle \subseteq R_j$ are taken from Lemma 2.7.17, Lemma 2.7.19 and Corollary 2.7.22 respectively. In addition, set $J_{\ell,j}^\dagger := \emptyset$ and $P_{\ell,j}^\dagger := \emptyset$. It follows from Corollary 2.7.22 that $P_{i+1,\,j}^\dagger \subseteq P_{i,j}^\dagger \subseteq J_{i,j}^\dagger \subseteq R_j^\dagger$ for all $1 \leq i \leq \ell - 1$, so

$$R_j^\dagger = \bigl(R_j^\dagger \setminus \operatorname{Int} P_{1,j}^\dagger\bigr) \cup \textstyle\bigcup_{i=1}^{\ell-1} \bigl(P_{i,j}^\dagger \setminus \operatorname{Int} P_{i+1,\,j}^\dagger\bigr). \tag{2.6.41}$$

By our choice of ℓ, the interiors of $(R_j^\dagger \setminus \operatorname{Int} P_{1,j}^\dagger), (P_{1,j}^\dagger \setminus \operatorname{Int} P_{2,j}^\dagger), \ldots, (P_{\ell-1,\,j}^\dagger \setminus \operatorname{Int} P_{\ell,j}^\dagger)$ are non-empty and pairwise disjoint, and by Corollary 2.7.22(ii), each of these ℓ sets can be expressed as the union of $\lesssim \log^{d-1}(1/\delta)$ d-simplices with pairwise disjoint interiors. Moreover, defining $Q^\triangle$ as in Lemma 2.7.19 and J_η as in Lemma 2.7.17 for $\eta > 0$, we can apply Corollary 2.7.22(i), Lemma 2.7.19 and Lemma 2.7.17(iii) in that order to deduce that

$$\mu_d(R_j^\dagger \setminus P_{i,j}^\dagger) \lesssim \mu_d(R_j^\dagger \setminus J_{i,j}^\dagger) \lesssim \mu_d(Q^\triangle \setminus J_{4^i\delta^2}) \lesssim \mu_d([0,1/2]^d \setminus J_{4^i\delta^2}) \lesssim 4^i\delta^2 \log^{d-1}(1/\delta) \tag{2.6.42}$$

for all $1 \leq i \leq \ell$. It follows that $\mu_d(P_{i,j}^\dagger \setminus P_{i+1,\,j}^\dagger) \leq \mu_d(R_j^\dagger \setminus P_{i+1,\,j}^\dagger) \lesssim 4^i\delta^2 \log^{d-1}(1/\delta)$ for all $1 \leq i \leq \ell - 1$. We emphasise here that the hidden multiplicative constants in these bounds do not depend on i.

Now if $f \in \mathcal{G}(f_S, \delta)$, then Lemma 2.7.14(ii) implies that $\log f \leq 2^{7/2}d\delta - \log \mu_d(S) \leq 2^{7/2}d\,(d+1)^{-d/2} - \log \mu_d(S)$ on S. Also, for each $1 \leq i \leq \ell - 1$, we deduce from Lemma 2.7.19(iii) that $\log f(x) \geq -2^{-i+2}(d!)^{-1/2} - \log \mu_d(S) \geq -2^{-i+2} - \log \mu_d(S)$ for all $x \in P_{i,j}^\dagger \setminus \operatorname{Int} P_{i+1,\,j}^\dagger \subseteq J_{i,j}^\dagger$. Thus, for each $1 \leq i \leq \ell - 1$, it follows from the observations above and (2.6.33) from Proposition 2.6.7 that

$$\begin{aligned} H_{[\,]}\bigl(\varepsilon'/\sqrt{\ell}, \mathcal{G}(f_S,\delta), d_{\mathrm{H}}, P_{i,j}^\dagger \setminus P_{i+1,\,j}^\dagger\bigr) &\lesssim \log^{d-1}\biggl(\frac{1}{\delta}\biggr)\biggl(\frac{(2^{7/2}d\delta + 2^{-i+2})\{4^i\delta^2\log^{d-1}(1/\delta)\}^{1/2}}{\ell^{-1/2}\,\varepsilon}\biggr)^{d/2} \\ &\lesssim \biggl(\frac{\delta}{\varepsilon}\biggr)^{d/2} \log^{\frac{d(d+4)}{4}-1}\biggl(\frac{1}{\delta}\biggr)\,\bigl(2^{7/2}d\,(2^i\delta) + 4\bigr)^{d/2} \\ &\lesssim \biggl(\frac{\delta}{\varepsilon}\biggr)^{d/2} \log^{\frac{d(d+4)}{4}-1}\biggl(\frac{1}{\delta}\biggr), \end{aligned}$$

where the final bound follows from the fact that $2^i\delta \leq 2^{\ell-1}\delta \leq (d+1)^{-d/2} \leq 2^{-d/2}$. Since $1 \leq \ell \lesssim \log(1/\delta)$ and the hidden multiplicative constants in the bounds above do not depend on i, we conclude that

$$\begin{aligned} H_{[\,]}\bigl(\varepsilon', \mathcal{G}(f_S,\delta), d_{\mathrm{H}}, P_{1,j}^\dagger\bigr) &\leq \sum_{i=1}^{\ell-1} H_{[\,]}\bigl(\varepsilon'/\sqrt{\ell}, \mathcal{G}(f_S,\delta), d_{\mathrm{H}}, P_{i,j}^\dagger \setminus P_{i+1,\,j}^\dagger\bigr) \\ &\lesssim \biggl(\frac{\delta}{\varepsilon}\biggr)^{d/2} \log^{\frac{d(d+4)}{4}}\biggl(\frac{1}{\delta}\biggr). \end{aligned} \tag{2.6.43}$$

Furthermore, recalling that every $f \in \mathcal{G}(f_S, \delta)$ satisfies $f \leq e^{2^{7/2}d\delta - \log \mu_d(S)} \lesssim 1$ on $R_j^\dagger \setminus \operatorname{Int} P_{1,j}^\dagger$, we may apply the final assertion of Proposition 2.6.7 together with (2.6.42) to deduce that

$$H_{[\,]}\bigl(\varepsilon', \mathcal{G}(f_S,\delta), d_{\mathrm{H}}, R_j^\dagger \setminus P_{1,j}^\dagger\bigr) \lesssim \log^{d-1}\biggl(\frac{1}{\delta}\biggr)\, h_d\biggl(\frac{\varepsilon}{\delta\log^{(d-1)/2}(1/\delta)}\biggr). \tag{2.6.44}$$

Having now established (2.6.43) and (2.6.44) for each fixed $1 \le j \le d+1$, we finally note that

$$H_{[\,]}\big(2^{1/2}\varepsilon, \mathcal{G}(f_S,\delta), d_{\mathrm{H}}\big) \le \sum_{j=1}^{d+1} \big\{H_{[\,]}(\varepsilon', \mathcal{G}(f_S,\delta), d_{\mathrm{H}}, R_j^\dagger \setminus P_{1,j}^\dagger) + H_{[\,]}(\varepsilon', \mathcal{G}(f_S,\delta), d_{\mathrm{H}}, P_{1,j}^\dagger)\big\}. \quad (2.6.45)$$

Thus, when $d = 2$, we conclude that

$$H_{[\,]}\big(2^{1/2}\varepsilon, \mathcal{G}(f_S,\delta), d_{\mathrm{H}}\big) \lesssim \left(\frac{\delta}{\varepsilon}\right) \log^{3/2}\left(\frac{1}{\delta}\right) \left\{\log^{3/2}\left(\frac{1}{\delta}\right) + \log^{3/2}\left(\frac{\delta \log^{1/2}(1/\delta)}{\varepsilon}\right)\right\}, \quad (2.6.46)$$

which is bounded above by the quantity $H_2(\delta,\varepsilon)$ in (2.6.39) up to a universal constant. Similarly, when $d = 3$, the bound (2.6.40) follows immediately on combining (2.6.43), (2.6.44) and (2.6.45). $\square$

We now extend Proposition 2.6.8 to the case where f_0 is the uniform density f_K on a polytope $K \in \mathcal{P}^m$. By Lemma 2.7.11, every polytope in $\mathcal{P}_d$ has at least as many facets as a d-simplex, namely $d+1$.

Proposition 2.6.9. *Let $d \in \{2,3\}$ and fix $m \in \mathbb{N}$ with $m \ge d+1$. If $0 < \varepsilon < \delta < 2^{-3/2}$ and $K \in \mathcal{P}^m$ is a polytope, then*

$$H_{[\,]}\big(2^{1/2}\varepsilon, \mathcal{G}(f_K,\delta), d_{\mathrm{H}}\big) \lesssim m \left(\frac{\delta}{\varepsilon}\right) \log^{3/2}\left(\frac{1}{\delta}\right) \log^{3/2}\left(\frac{\log(1/\delta)}{\varepsilon}\right) = mH_2(\delta,\varepsilon) \quad (2.6.47)$$

when $d = 2$ and

$$H_{[\,]}\big(2^{1/2}\varepsilon, \mathcal{G}(f_K,\delta), d_{\mathrm{H}}\big) \lesssim m \left\{\left(\frac{\delta}{\varepsilon}\right)^2 \log^4\left(\frac{1}{\delta}\right) + \left(\frac{\delta}{\varepsilon}\right)^{3/2} \log^{21/4}\left(\frac{1}{\delta}\right)\right\} = mH_3(\delta,\varepsilon) \quad (2.6.48)$$

when $d = 3$.

Proof. Fix $d \in \{2,3\}$ and suppose that $0 < \varepsilon < \delta < 2^{-3/2}$. By Proposition 2.7.12, we can find $M \le 6m$ d-simplices $S_1, \dots, S_M$ with pairwise disjoint interiors whose union is K. Set $\alpha_j := \{\mu_d(S_j)/\mu_d(K)\}^{1/2}$ for each $1 \le j \le M$, so that $\sum_{j=1}^M \alpha_j^2 = 1$. For each $f \in \mathcal{G}(f_K,\delta)$ and $1 \le j \le M$, let $n_j(f)$ be the smallest $n_j \in \mathbb{N}$ for which $\int_{S_j} \big(\sqrt{f} - \sqrt{f_K}\big)^2 \le \alpha_j^2\, n_j \delta^2$. By the minimality of $n_j(f)$, we have $\alpha_j^2\,(n_j(f) - 1)\,\delta^2 \le \int_{S_j} \big(\sqrt{f} - \sqrt{f_K}\big)^2$ for each j, so

$$\begin{aligned}\sum_{j=1}^M \alpha_j^2\, n_j(f) = 1 + \sum_{j=1}^M \alpha_j^2\,(n_j(f) - 1) &\le 1 + \delta^{-2} \sum_{j=1}^M \int_{S_j} \big(\sqrt{f} - \sqrt{f_K}\big)^2 \\ &= 1 + \delta^{-2} \int_K \big(\sqrt{f} - \sqrt{f_K}\big)^2 \le 2, \end{aligned} \quad (2.6.49)$$

where the final inequality follows because $f \in \mathcal{G}(f_K,\delta)$. We also claim that $n_j(f) \lesssim \delta^{-2}$ for all $1 \le j \le M$. To see this, note that since $f \in \mathcal{G}(f_K,\delta)$ and $\delta < 2^{-3/2}$, it follows from Lemma 2.7.14(ii) that

$$0 \le f \le e^{8\sqrt{2}d\delta} f_K \le e^{4d} f_K = e^{4d} \mu_d(K)^{-1} \ \text{ on } K. \quad (2.6.50)$$

Thus, we have $\big(\sqrt{f} - \sqrt{f_K}\big)^2 \le f \vee f_K \lesssim f_K = \mu_d(K)^{-1}$ on K, so $\int_{S_j} \big(\sqrt{f} - \sqrt{f_K}\big)^2 \lesssim \mu_d(S_j)/\mu_d(K) = \alpha_j^2$ for all j. Recalling the definition of $n_j(f)$, we deduce that $n_j(f) \lesssim \delta^{-2}$ for all j, as required.

Now let $U := \{(n_1(f), \dots, n_M(f)) : f \in \mathcal{G}(f_K,\delta)\}$, and for each $(n_1, \dots, n_M) \in U$, define

$$\mathcal{G}(f_K, \delta; n_1, \dots, n_M) := \{f \in \mathcal{G}(f_K,\delta) : n_j(f) = n_j \text{ for all } 1 \le j \le M\}.$$

Since $\mathcal{G}(f_K,\delta)$ is the union of these subclasses, it follows that

$$N_{[]}\bigl(2^{1/2}\varepsilon,\mathcal{G}(f_K,\delta),d_{\mathrm{H}}\bigr) \leq \sum_{(n_1,\ldots,n_M)\in U} N_{[]}\bigl(2^{1/2}\varepsilon,\mathcal{G}(f_K,\delta;n_1,\ldots,n_M),d_{\mathrm{H}}\bigr),$$

so

$$H_{[]}\bigl(2^{1/2}\varepsilon,\mathcal{G}(f_K,\delta),d_{\mathrm{H}}\bigr) \leq \log|U| + \max_{(n_1,\ldots,n_M)\in U} H_{[]}\bigl(2^{1/2}\varepsilon,\mathcal{G}(f_K,\delta;n_1,\ldots,n_M),d_{\mathrm{H}}\bigr). \tag{2.6.51}$$

Since $n_j(f) \lesssim \delta^{-2}$ for all $1 \leq j \leq M$, we deduce that $|U| \lesssim \delta^{-2M}$ and hence that

$$\log|U| \lesssim M\log(1/\delta) \lesssim m\log(1/\delta). \tag{2.6.52}$$

Next, we bound the second term on the right hand side of (2.6.51). Fix $j \in \{1,\ldots,M\}$ and $(n_1,\ldots,n_M) \in U$. If $f \in \mathcal{G}(f_K,\delta;n_1,\ldots,n_M)$, then $f_K\mathbb{1}_{S_j} = \alpha_j^2 f_{S_j}$ and $\int_{S_j}\bigl(\sqrt{f}-\sqrt{f_K}\bigr)^2 \leq \alpha_j^2 n_j\delta^2$, so $\int_{S_j}\bigl\{(\alpha_j^{-2}f)^{1/2}-f_{S_j}^{1/2}\bigr\}^2 \leq n_j\delta^2$. This shows that $\alpha_j^{-2}f\mathbb{1}_{S_j} \in \mathcal{G}(f_{S_j},\sqrt{n_j}\,\delta)$. In addition, it follows from (2.6.50) that

$$0 \leq \alpha_j^{-2}f\mathbb{1}_{S_j} = \mu_d(K)f\mathbb{1}_{S_j}/\mu_d(S_j) \leq e^{4d}\mu_d(S_j)^{-1}\mathbb{1}_{S_j} = e^{4d}f_{S_j} \text{ on } S_j. \tag{2.6.53}$$

Suppose first that $\sqrt{n_j}\,\delta < (d+1)^{-d/2}$. Since $0 < \sqrt{n_j}\,\varepsilon < \sqrt{n_j}\,\delta < (d+1)^{-d/2}$, we can apply Proposition 2.6.8 to deduce that there exists a $\sqrt{n_j}\,\varepsilon$-Hellinger bracketing set $\{[g_\ell^L,g_\ell^U] : 1 \leq \ell \leq N_j\}$ for $\mathcal{G}(f_{S_j},\sqrt{n_j}\,\delta)$ such that

$$\log N_j \lesssim H_d(\sqrt{n_j}\,\delta,\sqrt{n_j}\,\varepsilon) \lesssim H_d(\delta,\varepsilon).$$

Note that we can find $1 \leq \ell \leq N_j$ such that $g_\ell^L(x) \leq \alpha_j^{-2}f(x) \leq g_\ell^U(x)$ for all $x \in S_j$. Therefore, $\{f\mathbb{1}_{S_j} : f \in \mathcal{G}(f_K,\delta;n_1,\ldots,n_M)\}$ is covered by the brackets $\{[\alpha_j^2 g_\ell^L,\alpha_j^2 g_\ell^U] : 1 \leq \ell \leq N_j\}$. Since

$$\int_{S_j}\Bigl(\sqrt{\alpha_j^2 g_\ell^U}-\sqrt{\alpha_j^2 g_\ell^L}\Bigr)^2 = \alpha_j^2\int_{S_j}\Bigl(\sqrt{g_\ell^U}-\sqrt{g_\ell^L}\Bigr)^2 \leq \alpha_j^2 n_j\,\varepsilon^2 \tag{2.6.54}$$

for all $1 \leq \ell \leq N_j$, we conclude that

$$H_{[]}\bigl(\alpha_j\sqrt{n_j}\,\varepsilon,\mathcal{G}(f_K,\delta;n_1,\ldots,n_M),d_{\mathrm{H}},S_j\bigr) \lesssim H_d(\delta,\varepsilon), \tag{2.6.55}$$

provided that $\sqrt{n_j}\,\delta < (d+1)^{-d/2}$.

We now verify that (2.6.55) remains valid when $\sqrt{n_j}\,\delta \geq (d+1)^{-d/2}$. In this case, we define $B_j := 4d\log(\mu_d(S_j)^{-1})$ and deduce from (2.6.53) that $\{\alpha_j^{-2}f\mathbb{1}_{S_j} : f \in \mathcal{G}(f_K,\delta;n_1,\ldots,n_M)\} \subseteq \mathcal{G}_{-\infty,B_j}(S_j)$. By the final bound (2.6.35) from Proposition 2.6.7, we can find a $\sqrt{n_j}\,\varepsilon$-Hellinger bracketing set $\{[\tilde{g}_\ell^L,\tilde{g}_\ell^U] : 1 \leq \ell \leq \tilde{N}_j\}$ for $\mathcal{G}_{-\infty,B_j}(S_j)$ such that

$$\log\tilde{N}_j \lesssim h_d\biggl(\frac{\sqrt{n_j}\,\varepsilon}{e^{B_j/2}\mu_d(S_j)^{1/2}}\biggr) = h_d\biggl(\frac{\sqrt{n_j}\,\varepsilon}{e^{2d}}\biggr) \lesssim h_d\Bigl(\frac{\varepsilon}{\delta}\Bigr) \lesssim H_d(\delta,\varepsilon).$$

Indeed, the penultimate inequality above follows since $\sqrt{n_j}\,\delta \geq (d+1)^{-d/2} \gtrsim 1$ and h_d is decreasing, and the final inequality can be verified separately for $d = 2,3$; see (2.6.46) for example to obtain the bound when $d = 2$. As above, we see that $\{f\mathbb{1}_{S_j} : f \in \mathcal{G}(f_K,\delta;n_1,\ldots,n_M)\}$ is covered by the brackets $\{[\alpha_j^2\,\tilde{g}_\ell^L, \alpha_j^2\,\tilde{g}_\ell^U] : 1 \leq \ell \leq \tilde{N}_j\}$, and as in (2.6.54), we have

$$\int_{S_j}\biggl(\sqrt{\alpha_j^2\,\tilde{g}_\ell^U} - \sqrt{\alpha_j^2\,\tilde{g}_\ell^L}\biggr)^2 \leq \alpha_j^2\, n_j\, \varepsilon^2$$

for all j. It follows that

$$H_{[\,]}\bigl(\alpha_j\sqrt{n_j}\,\varepsilon, \mathcal{G}(f_K, \delta; n_1, \dots, n_M), d_{\mathrm{H}}, S_j\bigr) \leq \log \tilde{N}_j \lesssim H_d(\delta, \varepsilon),$$

so (2.6.55) holds when $\sqrt{n_j}\,\delta \geq (d+1)^{-d/2}$, as required.

Finally, since $(n_1, \dots, n_M) \in U$, it follows from (2.6.49) and the definition of U above that $\sum_{j=1}^M \alpha_j^2\, n_j\, \varepsilon^2 \leq 2\varepsilon^2$. Having established (2.6.55) for all $1 \leq j \leq M$, we conclude that

$$\begin{aligned} H_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_K, \delta; n_1, \dots, n_M), d_{\mathrm{H}}\bigr) &\leq \sum_{j=1}^M H_{[\,]}\bigl(\alpha_j\sqrt{n_j}\,\varepsilon, \mathcal{G}(f_K, \delta; n_1, \dots, n_M), d_{\mathrm{H}}, S_j\bigr) \\ &\lesssim M H_d(\delta, \varepsilon) \lesssim m H_d(\delta, \varepsilon) \end{aligned}$$

whenever $0 < \varepsilon < \delta < 2^{-3/2}$ and $(n_1, \dots, n_M) \in U$. Together with (2.6.51) and (2.6.52), this implies the desired conclusion. □

Turning now to the subclasses $\mathcal{F}^{[\theta]}(\mathcal{P}^m)$ defined in Section 2.3, we first establish an analogue of Proposition 2.6.8.

Proposition 2.6.10. *Let $d = 3$ and let $S \subseteq \mathbb{R}^3$ be a 3-simplex. If $0 < \varepsilon < \delta < 2^{-3}\,\theta^{-1/2}$ and $f_0 \in \mathcal{F}^{[\theta]}(S) \equiv \mathcal{F}_3^{[\theta]}(S)$ for some $\theta \in (1, \infty)$, then*

$$\begin{aligned} H_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0, \delta), d_{\mathrm{H}}\bigr) \lesssim \frac{\log^{3/2}\theta + \delta^{3/5}}{\varepsilon^{3/2}} \log^{17/4}\biggl(\frac{1}{\theta\delta^2}\biggr) + \theta^{3/4}\biggl(\frac{\delta}{\varepsilon}\biggr)^{3/2} \log^{21/4}\biggl(\frac{1}{\theta\delta^2}\biggr) \\ + \theta\log^3(e\theta)\biggl(\frac{\delta}{\varepsilon}\biggr)^2 \log^4\biggl(\frac{1}{\theta\delta^2}\biggr) \qquad (2.6.56) \\ =: H_{3,\theta}(\delta, \varepsilon). \end{aligned}$$

The following proof is similar in structure and content to that of Proposition 2.6.8, although alterations must be made to the arguments that previously relied on the pointwise upper bound from Lemma 2.7.14(ii), which applies only when f_0 is uniform. For general $\theta \in (1, \infty)$ and $f_0 \in \mathcal{F}^{[\theta]}(S)$, we instead turn to Lemma 2.7.14(iii) for a pointwise upper bound on functions $f \in \mathcal{G}(f_0, \delta)$. While the bound in Lemma 2.7.14(ii) features a term of order δ, the corresponding term in Lemma 2.7.14(iii) is of order $\delta^{2/(d+2)} = \delta^{2/5}$ when $d = 3$. The latter manifests itself in the overall bound (2.6.56) through the contribution of order $(\delta^{2/5}/\varepsilon)^{3/2}\log^{17/4}\bigl(1/(\theta\delta^2)\bigr)$, which in turn is ultimately responsible for the term of order $(m/n)^{20/29}\log^{85/29} n$ in the adaptive risk bound (2.3.1) in Theorem 2.3.1. This explains why we do not recover the local bracketing entropy bounds (2.6.40) and (2.6.48) in Propositions 2.6.8 and 2.6.9 or the risk bound (2.2.4) in Proposition 2.2.4 when we take the limit $\theta \searrow 1$ in (2.6.56), (2.6.60) and (2.3.1) respectively.

On the other hand, since $f_0 \in \mathcal{F}^{[\theta]}(S)$ is bounded below by $\theta^{-1} f_S$ (and hence bounded away from 0) on S, the pointwise lower bound on $f \in \mathcal{G}(f_0, \delta)$ from Lemma 2.7.14(i) can still be applied in this context. By extension, the same is true of the constructions and reasoning based on Corollary 2.7.22 and Lemmas 2.7.17 and 2.7.19. As such, we will reuse much of the notation from the proof of Proposition 2.6.8, and we will also repeat many of the key definitions and intermediate assertions without further justification or explanation.

Proof. Suppose that $0 < \varepsilon < \delta < 2^{-3}\,\theta^{-1/2}$. Let $\varepsilon' := \varepsilon/\sqrt{d+1} = \varepsilon/2$ and $\ell := \lceil \log_2(\theta^{-1/2}\delta^{-1}/8)\rceil$, so that ℓ is the smallest integer i such that $4^i\theta\delta^2 \geq 4^{-3} = (d+1)^{-d}$, and note that $1 \leq \ell \lesssim \log\bigl(1/(\theta\delta^2)\bigr)$. As in the proof of Proposition 2.6.8, we may assume without loss of generality that S is a regular 3-simplex with side length $\sqrt{2}$. Once again, let $T\colon \operatorname{aff}\triangle \to \mathbb{R}^3$ be an affine isometry such that $T(\triangle) = S$, and define $R_j^\dagger := T(R_j)$ for $1 \leq j \leq d+1 = 4$, so that $R_1^\dagger, \ldots, R_4^\dagger$ are polytopes with disjoint interiors whose union is S.

For a fixed $j \in \{1, \ldots, 4\}$, we now follow closely the second paragraph of the proof of Proposition 2.6.8 and construct a family of nested polytopes within $R_j^\dagger$. For each $i \in \{1, \ldots, \ell-1\}$, define $J_{i,j}^\dagger := T\bigl(R_j \cap J_{4^i\theta\delta^2}^\triangle\bigr)$ and $P_{i,j}^\dagger := T\bigl(P_{4^i\theta\delta^2,\,j}^\triangle\bigr)$. In addition, let $J_{\ell,j}^\dagger := \emptyset$ and $P_{\ell,j}^\dagger := \emptyset$. Then $P_{i+1,\,j}^\dagger \subseteq P_{i,j}^\dagger \subseteq J_{i,j}^\dagger \subseteq R_j^\dagger$ for all $1 \leq i \leq \ell-1$, and as in (2.6.41), we can write $R_j^\dagger$ as the union of $(R_j^\dagger \setminus \operatorname{Int} P_{1,j}^\dagger), (P_{1,j}^\dagger \setminus \operatorname{Int} P_{2,j}^\dagger), \ldots, (P_{\ell-1,\,j}^\dagger \setminus \operatorname{Int} P_{\ell,j}^\dagger)$, whose interiors are non-empty and pairwise disjoint. Each of these ℓ sets may be expressed as the union of $\lesssim \log^2\bigl(1/(\theta\delta^2)\bigr)$ 3-simplices with pairwise disjoint interiors, and similarly to (2.6.42), we have

$$\mu_3(R_j^\dagger \setminus P_{i,j}^\dagger) \lesssim \mu_3(R_j^\dagger \setminus J_{i,j}^\dagger) \lesssim \mu_3(Q^\triangle \setminus J_{4^i\theta\delta^2}) \lesssim \mu_3([0,1/2]^3 \setminus J_{4^i\theta\delta^2}) \lesssim 4^i\theta\delta^2\log^2\bigl(1/(\theta\delta^2)\bigr) \tag{2.6.57}$$

for all $1 \leq i \leq \ell$. Thus, $\mu_3(P_{i,j}^\dagger \setminus P_{i+1,\,j}^\dagger) \leq \mu_3(R_j^\dagger \setminus P_{i+1,\,j}^\dagger) \lesssim 4^i\theta\delta^2\log^2\bigl(1/(\theta\delta^2)\bigr)$ for all $1 \leq i \leq \ell-1$. We emphasise again that the hidden multiplicative constants in these bounds do not depend on i.

Now let the universal constants $s_3 \geq 1$ and $s' > 0$ be as in Lemma 2.7.14(iii). For $\tilde{\theta} \in [1,\infty)$, define $t(\tilde{\theta}) \equiv t_3(\tilde{\theta}) = \log(s_3\log^3(e\tilde{\theta}) - s_3 + 1)$ as in the proof of this result, and note that $t(\tilde{\theta}) \lesssim \log\tilde{\theta}$ and $e^{t(\tilde{\theta})} \lesssim \log^3(e\tilde{\theta})$. If $f \in \mathcal{G}(f_0,\delta)$, then it follows from Lemma 2.7.14(iii) that $\log f \leq t(\theta) + s'(3^4\delta)^{2/5} - \log\mu_3(S)$ on S. Also, for each $1 \leq i \leq \ell-1$, we deduce from Lemma 2.7.19(iii) that $\log f(x) \geq -2^{-i+2}(3!)^{-1/2} - \log\theta - \log\mu_3(S) \geq -2^{-i+2} - \log\theta - \log\mu_3(S)$ for all $x \in P_{i,j}^\dagger \setminus \operatorname{Int} P_{i+1,\,j}^\dagger \subseteq J_{i,j}^\dagger$. Thus, for each $1 \leq i \leq \ell-1$, it follows from the observations above and (2.6.33) from Proposition 2.6.7 that

$$\begin{aligned}
&H_{[\,]}\bigl(\varepsilon'/\sqrt{\ell}, \mathcal{G}(f_0,\delta), d_{\mathrm{H}}, P_{i,j}^\dagger \setminus P_{i+1,\,j}^\dagger\bigr)\\
&\quad\lesssim \log^2\biggl(\frac{1}{\theta\delta^2}\biggr)\left(\frac{\bigl\{\log\theta + t(\theta) + s'(3^4\delta)^{2/5} + 2^{-i+2}\bigr\}\bigl\{4^i\theta\delta^2\log^2\bigl(1/(\theta\delta^2)\bigr)\bigr\}^{1/2}}{\ell^{-1/2}\,\varepsilon}\right)^{3/2}\\
&\quad\lesssim \left(\frac{\delta}{\varepsilon}\right)^{3/2}\log^{17/4}\left(\frac{1}{\theta\delta^2}\right)\theta^{3/4}\left(2^i\log\theta + 2^i\delta^{2/5} + 4\right)^{3/2}\\
&\quad\lesssim \left(\frac{\delta}{\varepsilon}\right)^{3/2}\log^{17/4}\left(\frac{1}{\theta\delta^2}\right)\theta^{3/4}\left(2^{3i/2}\log^{3/2}\theta + 2^{3i/2}\delta^{3/5} + 1\right).
\end{aligned}$$

By our choice of ℓ, we have $\ell \lesssim \log\bigl(1/(\theta\delta^2)\bigr)$ and $\sum_{i=1}^{\ell-1} 2^{3i/2} \lesssim 2^{3(\ell-1)/2} - 1 \lesssim (\theta\delta^2)^{-3/4}$, and since $\theta > 1$ and $\theta\delta^2 < 2^{-3}$, we conclude that

$$\begin{aligned}
H_{[\,]}\bigl(\varepsilon', \mathcal{G}(f_0,\delta), d_{\mathrm{H}}, P_{1,j}^\dagger\bigr) &\leq \sum_{i=1}^{\ell-1} H_{[\,]}\bigl(\varepsilon'/\sqrt{\ell}, \mathcal{G}(f_0,\delta), d_{\mathrm{H}}, P_{i,j}^\dagger \setminus P_{i+1,\,j}^\dagger\bigr)\\
&\lesssim \frac{1}{\varepsilon^{3/2}}\log^{17/4}\left(\frac{1}{\theta\delta^2}\right)\left(\log^{3/2}\theta + \delta^{3/5} + (\theta\delta^2)^{3/4}\,\ell\right)\\
&\lesssim \frac{1}{\varepsilon^{3/2}}\log^{17/4}\left(\frac{1}{\theta\delta^2}\right)\left(\log^{3/2}\theta + \delta^{3/5}\right) + \theta^{3/4}\left(\frac{\delta}{\varepsilon}\right)^{3/2}\log^{21/4}\left(\frac{1}{\theta\delta^2}\right).
\end{aligned} \tag{2.6.58}$$

Furthermore, recalling that every $f \in \mathcal{G}(f_0,\delta)$ satisfies $f \leq e^{t(\theta)+s'(3^4\delta)^{2/5}-\log\mu_3(S)} \lesssim e^{t(\theta)} \lesssim \log^3(e\theta)$ on $R_j^\dagger \setminus \operatorname{Int} P_{1,j}^\dagger$, we may apply the final assertion of Proposition 2.6.7 together with (2.6.57) to deduce that

$$H_{[\,]}\bigl(\varepsilon', \mathcal{G}(f_0,\delta), d_{\mathrm{H}}, R_j^\dagger \setminus P_{1,j}^\dagger\bigr) \lesssim \log^2\biggl(\frac{1}{\theta\delta^2}\biggr)\frac{\theta\delta^2\log^2\bigl(1/(\theta\delta^2)\bigr)\log^3(e\theta)}{\varepsilon^2}$$
$$\lesssim \theta\log^3(e\theta)\biggl(\frac{\delta}{\varepsilon}\biggr)^2\log^4\biggl(\frac{1}{\theta\delta^2}\biggr). \tag{2.6.59}$$

Now that we have established (2.6.58) and (2.6.59) for each $1 \leq j \leq d+1 = 4$, the result follows on noting that

$$H_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0,\delta), d_{\mathrm{H}}\bigr) \leq \sum_{j=1}^{4}\bigl\{H_{[\,]}\bigl(\varepsilon', \mathcal{G}(f_0,\delta), d_{\mathrm{H}}, R_j^\dagger \setminus P_{1,j}^\dagger\bigr) + H_{[\,]}\bigl(\varepsilon', \mathcal{G}(f_0,\delta), d_{\mathrm{H}}, P_{1,j}^\dagger\bigr)\bigr\}.$$

□

By imitating the proof of Proposition 2.6.9, we obtain the key local bracketing entropy result that enables us to prove Theorem 2.3.1.

Proposition 2.6.11. *Let $d = 3$ and fix $\theta \in (1,\infty)$. If $0 < \varepsilon < \delta < (8\theta)^{-1/2}$ and $f_0 \in \mathcal{F}^{[\theta]}(\mathcal{P}^m)$ for some $m \geq 4$, then*

$$\begin{aligned} H_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0,\delta), d_{\mathrm{H}}\bigr) &\lesssim m\Biggl\{\frac{\log^{3/2}\theta + \delta^{3/5}}{\varepsilon^{3/2}}\log^{17/4}\biggl(\frac{1}{\theta\delta^2}\biggr) + \theta^{3/4}\biggl(\frac{\delta}{\varepsilon}\biggr)^{3/2}\log^{21/4}\biggl(\frac{1}{\theta\delta^2}\biggr) \\ &\qquad + \theta\log^3(e\theta)\biggl(\frac{\delta}{\varepsilon}\biggr)^2\log^4\biggl(\frac{1}{\theta\delta^2}\biggr)\Biggr\} \\ &= mH_{3,\theta}(\delta,\varepsilon). \end{aligned} \tag{2.6.60}$$

Proof. Suppose that $0 < \varepsilon < \delta < (8\theta)^{-1/2}$. By Proposition 2.7.12, we can find $M \leq 6m$ 3-simplices $S_1,\ldots,S_M$ with pairwise disjoint interiors whose union is $P := \operatorname{supp} f_0$. Set $\alpha_j := \{\mu_3(S_j)/\mu_3(P)\}^{1/2}$ for each $1 \leq j \leq M$, so that $\sum_{j=1}^M \alpha_j^2 = 1$. For each $f \in \mathcal{G}(f_0,\delta)$ and $1 \leq j \leq M$, let $n_j(f)$ be the smallest $n_j \in \mathbb{N}$ for which $\int_{S_j}\bigl(\sqrt{f} - \sqrt{f_0}\bigr)^2 \leq \alpha_j^2 n_j\delta^2$, so that $\sum_{j=1}^M \alpha_j^2 n_j(f) \leq 2$, as in (2.6.49). We also claim that $n_j(f) \lesssim \log^3(e\theta)\,\delta^{-2}$ for all $1 \leq j \leq M$. To see this, let $t(\theta) \equiv t_3(\theta)$ be as in the proof of Lemma 2.7.14 and note that since $f_0 \in \mathcal{F}^{[\theta]}(P)$, $\delta < (8\theta)^{-1/2}$ and $f \in \mathcal{G}(f_0,\delta)$, it follows from Lemma 2.7.14(iii) that

$$0 \leq f \vee f_0 \lesssim e^{t(\theta) - \log\mu_3(P)} \lesssim \log^3(e\theta)\,\mu_3(P)^{-1} = \log^3(e\theta)\,f_P \ \text{ on } P. \tag{2.6.61}$$

Thus, we have $\bigl(\sqrt{f} - \sqrt{f_0}\bigr)^2 \leq f \vee f_0 \lesssim \log^3(e\theta)\,f_P = \log^3(e\theta)\,\mu_3(P)^{-1}$ on P, so $\int_{S_j}\bigl(\sqrt{f} - \sqrt{f_0}\bigr)^2 \lesssim \log^3(e\theta)\,\mu_3(S_j)/\mu_3(P) = \log^3(e\theta)\,\alpha_j^2$ for all j. Recalling the definition of $n_j(f)$, we deduce that $n_j(f) \lesssim \log^3(e\theta)\,\delta^{-2}$ for all j, as required.

Now let $U := \{(n_1(f),\ldots,n_M(f)) : f \in \mathcal{G}(f_0,\delta)\}$, and for each $(n_1,\ldots,n_M) \in U$, define

$$\mathcal{G}(f_0,\delta;n_1,\ldots,n_M) := \{f \in \mathcal{G}(f_0,\delta) : n_j(f) = n_j \text{ for all } 1 \leq j \leq M\}.$$

Since $\mathcal{G}(f_0,\delta)$ is the union of these subclasses, it follows that

$$N_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0,\delta), d_{\mathrm{H}}\bigr) \leq \sum_{(n_1,\ldots,n_M)\in U} N_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0,\delta;n_1,\ldots,n_M), d_{\mathrm{H}}\bigr),$$

so

$$H_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0,\delta), d_{\mathrm{H}}\bigr) \leq \log|U| + \max_{(n_1,\ldots,n_M)\in U} H_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0,\delta;n_1,\ldots,n_M), d_{\mathrm{H}}\bigr). \tag{2.6.62}$$

Since $n_j(f) \lesssim \log^3(e\theta)\,\delta^{-2}$ for all $1 \leq j \leq M$, we deduce that $|U| \lesssim \log^{3M}(e\theta)\,\delta^{-2M}$ and hence that

$$\log|U| \lesssim M\bigl(\log\log(e\theta) + \log(1/\delta)\bigr) \lesssim m\bigl(\log\log(e\theta) + \log(1/\delta)\bigr). \tag{2.6.63}$$

Next, we bound the second term on the right hand side of (2.6.62). Fix $j \in \{1, \ldots, M\}$ and $(n_1, \ldots, n_M) \in U$. If $f \in \mathcal{G}(f_0, \delta; n_1, \ldots, n_M)$, then $\int_{S_j}\bigl(\sqrt{f} - \sqrt{f_0}\bigr)^2 \leq \alpha_j^2 n_j \delta^2$, so we have $\int_{S_j}\{(\alpha_j^{-2}f)^{1/2} - (\alpha_j^{-2}f_0)^{1/2}\}^2 \leq n_j\delta^2$. This shows that $\alpha_j^{-2}f\mathbb{1}_{S_j} \in \mathcal{G}(\alpha_j^{-2}f_0\mathbb{1}_{S_j}, \sqrt{n_j}\,\delta)$. Observe also that $\alpha_j^{-2}f_0\mathbb{1}_{S_j} \geq \theta^{-1}f_{S_j}$, whence $\alpha_j^{-2}f_0\mathbb{1}_{S_j} \in \mathcal{F}^{[\theta]}(S_j)$. Furthermore, it follows from (2.6.61) that

$$0 \leq \alpha_j^{-2}f\mathbb{1}_{S_j} = \mu_3(P)f\mathbb{1}_{S_j}/\mu_3(S_j) \lesssim \log^3(e\theta)\,\mu_3(S_j)^{-1}\mathbb{1}_{S_j} = \log^3(e\theta)\,f_{S_j} \text{ on } S_j. \tag{2.6.64}$$

Suppose first that $\sqrt{n_j}\,\delta < 2^{-3}\,\theta^{-1/2}$. Since $\alpha_j^{-2}f_0\mathbb{1}_{S_j} \in \mathcal{F}^{[\theta]}(S_j)$ and $0 < \sqrt{n_j}\,\varepsilon < \sqrt{n_j}\,\delta < 2^{-3}\,\theta^{-1/2}$, we can apply Proposition 2.6.10 to deduce that there exists a $\sqrt{n_j}\,\varepsilon$-Hellinger bracketing set $\{[g_\ell^L, g_\ell^U] : 1 \leq \ell \leq N_j\}$ for $\mathcal{G}(\alpha_j^{-2}f_0\mathbb{1}_{S_j}, \sqrt{n_j}\,\delta)$ such that

$$\log N_j \lesssim H_{3,\theta}(\sqrt{n_j}\,\delta, \sqrt{n_j}\,\varepsilon) \lesssim H_{3,\theta}(\delta, \varepsilon).$$

Arguing as in the proof of Proposition 2.6.9, we see that $\{[\alpha_j^2\,g_\ell^L, \alpha_j^2\,g_\ell^U] : 1 \leq \ell \leq N_j\}$ is an $(\alpha_j\sqrt{n_j}\,\varepsilon)$-Hellinger bracketing set for $\{f\mathbb{1}_{S_j} : f \in \mathcal{G}(f_0, \delta; n_1, \ldots, n_M)\}$, which implies that

$$H_{[\,]}\bigl(\alpha_j\sqrt{n_j}\,\varepsilon, \mathcal{G}(f_0, \delta; n_1, \ldots, n_M), d_{\mathrm{H}}, S_j\bigr) \lesssim H_{3,\theta}(\delta, \varepsilon), \tag{2.6.65}$$

provided that $\sqrt{n_j}\,\delta < 2^{-3}\,\theta^{-1/2}$.

We now verify that (2.6.65) remains valid even when $\sqrt{n_j}\,\delta \geq 2^{-3}\,\theta^{-1/2}$. In this case, we define $B_j := \log(\log^3(e\theta)\mu_3(S_j)^{-1})$ and deduce from (2.6.64) that for a sufficiently large universal constant $C > 0$, we have $\{\alpha_j^{-2}f\mathbb{1}_{S_j} : f \in \mathcal{G}(f_0, \delta; n_1, \ldots, n_M)\} \subseteq \mathcal{G}_{-\infty, CB_j}(S_j)$. By the final bound (2.6.35) from Proposition 2.6.7, we can find a $\sqrt{n_j}\,\varepsilon$-Hellinger bracketing set $\{[\tilde{g}_\ell^L, \tilde{g}_\ell^U] : 1 \leq \ell \leq \tilde{N}_j\}$ for $\mathcal{G}_{-\infty, CB_j}(S_j)$ such that

$$\log\tilde{N}_j \lesssim h_3\left(\frac{\sqrt{n_j}\,\varepsilon}{e^{B_j/2}\mu_3(S_j)^{1/2}}\right) \lesssim h_3\left(\frac{\sqrt{n_j}\,\varepsilon}{\log^{3/2}(e\theta)}\right) \lesssim h_3\left(\frac{\varepsilon}{\{\theta\log^3(e\theta)\}^{1/2}\,\delta}\right) \lesssim H_{3,\theta}(\delta, \varepsilon).$$

Indeed, the penultimate inequality above follows since $\sqrt{n_j}\,\delta \gtrsim \theta^{-1/2}$ and $h_3 \colon \eta \mapsto \eta^{-2}$ is decreasing, and the final inequality is easily verified. As above, we see that $\{[\alpha_j^2\,\tilde{g}_\ell^L, \alpha_j^2\,\tilde{g}_\ell^U] : 1 \leq \ell \leq \tilde{N}_j\}$ an $(\alpha_j\sqrt{n_j}\,\varepsilon)$-Hellinger bracketing set for $\{f\mathbb{1}_{S_j} : f \in \mathcal{G}(f_0, \delta; n_1, \ldots, n_M)\}$, which implies that

$$H_{[\,]}\bigl(\alpha_j\sqrt{n_j}\,\varepsilon, \mathcal{G}(f_0, \delta; n_1, \ldots, n_M), d_{\mathrm{H}}, S_j\bigr) \leq \log\tilde{N}_j \lesssim H_{3,\theta}(\delta, \varepsilon)$$

and hence that (2.6.65) holds when $\sqrt{n_j}\,\delta \geq 2^{-3}\,\theta^{-1/2}$, as required.

Finally, since $(n_1, \ldots, n_M) \in U$ and $\sum_{j=1}^M \alpha_j^2\,n_j(f) \leq 2$ for all $f \in \mathcal{G}(f_0, \delta)$, it follows from the definition of U that $\sum_{j=1}^M \alpha_j^2\,n_j\,\varepsilon^2 \leq 2\varepsilon^2$. Having established (2.6.65) for all $1 \leq j \leq M$, we conclude that

$$\begin{aligned} H_{[\,]}\bigl(2^{1/2}\varepsilon, \mathcal{G}(f_0, \delta; n_1, \ldots, n_M), d_{\mathrm{H}}\bigr) &\leq \sum_{j=1}^M H_{[\,]}\bigl(\alpha_j\sqrt{n_j}\,\varepsilon, \mathcal{G}(f_0, \delta; n_1, \ldots, n_M), d_{\mathrm{H}}, S_j\bigr) \\ &\lesssim MH_{3,\theta}(\delta, \varepsilon) \lesssim mH_{3,\theta}(\delta, \varepsilon) \end{aligned}$$

whenever $0 < \varepsilon < \delta < (8\theta)^{-1/2}$ and $(n_1, \ldots, n_M) \in U$. Together with (2.6.62) and (2.6.63), this implies the desired conclusion. $\square$

2.7 Technical preparation for Sections 2.2 and 2.6

2.7.1 Properties of log-concave, log-k-affine densities

The results in this section provide a basis for the definition of the complexity parameter $\Gamma(f)$ in Section 2.2, as well as for some important calculations in the derivation of the key local bracketing entropy bound (Proposition 2.5.1) in Section 2.5.1. Some of the propositions below are of independent interest; in particular, we obtain an explicit parametrisation of the subclass $\mathcal{F}^1$ of log-1-affine densities in $\mathcal{F}_d$ (Proposition 2.7.4) and also provide a proof of Proposition 2.2.1 in Section 2.2, which elucidates the geometric structure of log-concave, log-k-affine functions with polyhedral support. Much of the requisite convex analysis background and notation is set out in Section 1.4. The subclass $\mathcal{F}^1$ is not to be confused with the subclass $\mathcal{F}_1^{0,1}$ studied in Section 2.6.2.

To begin with, we state and prove two results from convex analysis, the second of which (Proposition 2.7.2) plays a crucial role in the subsequent theoretical development. A key ingredient in the proof of Proposition 2.7.2 is the powerful Brunn–Minkowski inequality (Schneider, 2014, Theorem 7.1.1).

Lemma 2.7.1. *Let $C \subseteq \mathbb{R}^d$ be a non-empty, closed, convex cone. Then we have the following:*

(i) $\operatorname{Int} C^* = \{\alpha \in \mathbb{R}^d : \alpha^\top x > 0$ *for all* $x \in C \setminus \{0\}\}$.

(ii) C *is pointed if and only if* $\operatorname{Int}(C^*)$ *is non-empty.*

This appears as Exercise B.16 in Ben-Tal and Nemirovski (2015), and we provide a proof here for convenience.

Proof. Let $h_C \colon \mathbb{R}^d \to \mathbb{R}$ be the function defined by $h_C(\alpha) := \inf\{\alpha^\top x : x \in C \cap S^{d-1}\}$, and observe that since $h_C(\alpha) \geq h_C(\alpha') + h_C(\alpha - \alpha')$ for all $\alpha, \alpha' \in \mathbb{R}^d$, it follows that h_C is in fact 1-Lipschitz with respect to the Euclidean norm. Indeed, we have

$$|h_C(\alpha) - h_C(\alpha')| \leq \max\{-h_C(\alpha - \alpha'), -h_C(\alpha' - \alpha)\} \leq \|\alpha - \alpha'\|$$

for all $\alpha, \alpha' \in \mathbb{R}^d$. Since h_C is positively homogeneous (i.e. $h_C(\lambda\alpha) = \lambda h_C(\alpha)$ for all $\lambda > 0$ and $\alpha \in \mathbb{R}^d$), we have $\alpha \in C^*$ if and only if $h_C(\alpha) \geq 0$. Now fix $\alpha \in \mathbb{R}^d$. If $\alpha^\top x > 0$ for all $x \in C \setminus \{0\}$, then since h_C is continuous and $C \cap S^{d-1}$ is compact, it follows that $h_C(\alpha) > 0$ and hence that $\alpha \in \operatorname{Int}(C^*)$. Conversely, if there exists $x \in C \setminus \{0\}$ such that $\alpha^\top x \leq 0$, then fix $v \in \mathbb{R}^d$ such that $\alpha^\top v < 0$ and note that $\alpha^\top(x + \varepsilon v) < 0$ for all $\varepsilon > 0$. This implies that $\alpha \notin \operatorname{Int}(C^*)$, so the proof of (i) is complete.

For (ii), observe that C^* has empty interior if and only if $\operatorname{span}(C^*)$ has dimension at most $d-1$, which is equivalent to saying that there exists $x \in \mathbb{R}^d \setminus \{0\}$ such that $\alpha^\top x = 0$ for all $\alpha \in C^*$. If this latter condition holds, then x and $-x$ both belong to $C^{**} = C$, so C is not pointed. On the other hand, if there exists $x \in \mathbb{R}^d \setminus \{0\}$ such that x and $-x$ lie in C, it follows from the definition of C^* that $\alpha^\top x = 0$ for all $\alpha \in C^*$, so the converse is also true. □

For $K \in \mathcal{K}$ and $\alpha \in \mathbb{R}^d$, let $m_{K,\alpha} := \inf_{x \in K} \alpha^\top x$ and $M_{K,\alpha} := \sup_{x \in K} \alpha^\top x$, and for each $t \in \mathbb{R}$, define the closed, convex sets

$$K_{\alpha,t}^+ := K \cap \{x \in \mathbb{R}^d : \alpha^\top x \leq t\} \quad \text{and} \quad K_{\alpha,t} := K \cap \{x \in \mathbb{R}^d : \alpha^\top x = t\}. \tag{2.7.1}$$

Proposition 2.7.2. *Let $K \in \mathcal{K}$ and $\alpha \in \mathbb{R}^d$. Then we have the following:*

(i) $K_{\alpha,t}^+$ *is compact for all* $t \in \mathbb{R}$ *if and only if* $\alpha \in \operatorname{Int}(\operatorname{rec}(K)^*)$.

(ii) If $\alpha \in \mathrm{Int}(\mathrm{rec}(K)^*) \setminus \{0\}$, then $m_{K,\alpha}$ is finite and $K_{\alpha,\, m_{K,\alpha}}$ is a non-empty exposed face of K. Moreover, if $d \geq 2$, then the function $t \mapsto \mu_{d-1}(K_{\alpha,t})^{1/(d-1)}$ is concave, finite-valued and strictly positive on $(m_{K,\alpha}, M_{K,\alpha})$.

Proof. (i) By taking $C := \mathrm{rec}(K)$ in Lemma 2.7.1(i), we see that

$$\mathrm{Int}(\mathrm{rec}(K)^*) = \bigl\{\alpha \in \mathbb{R}^d : \alpha^\top u > 0 \text{ for all } u \in \mathrm{rec}(K) \setminus \{0\}\bigr\}. \tag{2.7.2}$$

If $\alpha \notin \mathrm{Int}(\mathrm{rec}(K)^*)$, then there exists $u \in \mathrm{rec}(K) \setminus \{0\}$ such that $\alpha^\top u \leq 0$. Thus, if $K^+_{\alpha,t}$ is non-empty, then $x + \lambda u \in K$ and $\alpha^\top(x + \lambda u) \leq \alpha^\top x \leq t$ for all $x \in K^+_{\alpha,t}$ and $\lambda > 0$, so $K^+_{\alpha,t}$ is unbounded.

If $\alpha \in \mathrm{Int}(\mathrm{rec}(K)^*)$ and $t \in \mathbb{R}$ are such that $K^+_{\alpha,t}$ is non-empty, let $H^+ := \{u \in \mathbb{R}^d : \alpha^\top u > 0\}$ and $H^- := \{u \in \mathbb{R}^d : \alpha^\top u \leq 0\}$. Note that $\mathrm{rec}(K^+_{\alpha,t}) \setminus \{0\} \subseteq \mathrm{rec}(K) \setminus \{0\}$, which by (2.7.2) is disjoint from H^-. Moreover, if $x \in K^+_{\alpha,t}$ and $u \in H^+$, then there exists $\lambda > 0$ such that $\alpha^\top(x + \lambda u) > t$. Thus, since $x + \lambda u \notin K^+_{\alpha,t}$, it follows that $u \notin \mathrm{rec}(K^+_{\alpha,t})$. We conclude that $\mathrm{rec}(K^+_{\alpha,t}) = \{0\}$ and therefore that $K^+_{\alpha,t}$ is compact (Rockafellar, 1997, Theorem 8.4).

(ii) For $\alpha \in \mathrm{Int}(\mathrm{rec}(K)^*) \setminus \{0\}$, if we fix $y \in K^+_{\alpha,t}$ and set $s := \alpha^\top y$, then it follows from the compactness of $K^+_{\alpha,s}$ that

$$s \geq m_{K,\alpha} = \inf_{x \in K} \alpha^\top x = \inf_{x \in K^+_{\alpha,s}} \alpha^\top x > -\infty,$$

and that the infimum is attained at some $z \in K^+_{\alpha,s}$ with $\alpha^\top z = m_{K,\alpha}$. It is now clear that $K_{\alpha,\, m_{K,\alpha}}$ is a non-empty exposed face of K. Finally, if $d \geq 2$, fix $\lambda \in (0,1)$ and $t_1, t_2 \in \mathbb{R}$ with $m_{K,\alpha} \leq t_1 < t_2 \leq M_{K,\alpha}$, and set $t := \lambda t_1 + (1-\lambda)t_2$. Also, for $j = 1, 2$, fix $a_j \in K_{\alpha,t_j}$ and let $K'_j := K_{\alpha,t_j} - a_j$. Setting $a := \lambda a_1 + (1-\lambda)a_2 \in K_{\alpha,t}$, we see that $K' := K_{\alpha,t} - a$, K'_1 and K'_2 are contained in the $(d-1)$-dimensional subspace $H := \{u \in \mathbb{R}^d : \alpha^\top u = 0\}$. Since K^+_{α,t_2} is compact and convex, the sets $K_{\alpha,t}$, K_{α,t_1} and K_{α,t_2} are all non-empty and compact, and we have $K_{\alpha,t} \supseteq \lambda K_{\alpha,t_1} + (1-\lambda)K_{\alpha,t_2}$. This implies that $K' \supseteq \lambda K'_1 + (1-\lambda)K'_2$, so taking the ambient space to be H, we can apply the Brunn–Minkowski inequality (Schneider, 2014, Theorem 7.1.1) to deduce that

$$\begin{aligned}\mu_{d-1}(K_{\alpha,t})^{1/(d-1)} = \mu_{d-1}(K')^{1/(d-1)} &\geq \lambda \mu_{d-1}(K'_1)^{1/(d-1)} + (1-\lambda)\mu_{d-1}(K'_2)^{1/(d-1)} \\ &= \lambda \mu_{d-1}(K_{\alpha,t_1})^{1/(d-1)} + (1-\lambda)\mu_{d-1}(K_{\alpha,t_2})^{1/(d-1)}.\end{aligned}$$

Thus, $t \mapsto \mu_{d-1}(K_{\alpha,t})^{1/(d-1)}$ is indeed concave and finite-valued on $(m_{K,\alpha}, M_{K,\alpha})$. Since

$$0 < \mu_d(K) = \|\alpha\|^{-1} \int_{m_{K,\alpha}}^{M_{K,\alpha}} \mu_{d-1}(K_{\alpha,t})\, dt, \tag{2.7.3}$$

we deduce from this that $\mu_{d-1}(K_{\alpha,t}) > 0$ for all $t \in (m_{K,\alpha}, M_{K,\alpha})$, as required. To verify the identity (2.7.3), one can proceed as follows: let $\{u_1, \ldots, u_d\}$ be an orthonormal basis for $\mathbb{R}^d$ such that $u_d = \alpha/\|\alpha\|$, and let $Q \colon \mathbb{R}^d \to \mathbb{R}^d$ be the invertible linear map defined by setting $Qu_j = e_j$ for $j = 1, \ldots, d-1$ and $Qu_d = \|\alpha\| e_d$. Since $\det Q = \|\alpha\|$ and $\alpha^\top Q^{-1} w = \alpha^\top(w_d\, u_d/\|\alpha\|) = w_d$ for all $w = (w_1, \ldots, w_d) \in \mathbb{R}^d$, it follows that

$$\begin{aligned}\mu_d(K) &= \int_{Q(K)} \|\alpha\|^{-1}\, dw = \|\alpha\|^{-1} \int_{m_{K,\alpha}}^{M_{K,\alpha}} \mu_{d-1}(\{w \in Q^{-1}(K) : w_d = t\})\, dw_d \\ &= \|\alpha\|^{-1} \int_{m_{K,\alpha}}^{M_{K,\alpha}} \mu_{d-1}(K_{\alpha,t})\, dt,\end{aligned}$$

as claimed, where we have used Fubini's theorem to obtain the first equality. □

Next, we obtain a useful geometric characterisation of the sets $K \in \mathcal{K}$ for which $\mathrm{Int}(\mathrm{rec}(K)^*)$ is non-empty.

Proposition 2.7.3. *For a fixed $K \in \mathcal{K}$, the following are equivalent:*

(i) K is line-free; *(ii) $\mathrm{rec}(K)$ is a pointed cone;*

(iii) $\mathrm{Int}(\mathrm{rec}(K)^*)$ is non-empty; *(iv) K has at least one exposed point.*

Proof. (i) $\Leftrightarrow$ (ii): If K contains the line $L := \{y + \lambda u : \lambda \in \mathbb{R}\}$ and $x \in K$, then $x + \lambda u \in \mathrm{Cl}\,\mathrm{conv}\big(\{x\} \cup L\big) \subseteq K$ for every $\lambda \in \mathbb{R}$, so $\{\lambda u : \lambda \in \mathbb{R}\} \subseteq \mathrm{rec}(K)$. Therefore, $\mathrm{rec}(K)$ is not pointed. Conversely, if $\mathrm{rec}(K)$ is not pointed, then there exists $u \in \mathbb{R}^d \setminus \{0\}$ such that $u \in \mathrm{rec}(K) \cap (-\mathrm{rec}(K))$, so $K + \lambda u \subseteq K$ for all $\lambda \in \mathbb{R}$. Therefore, K is not line-free.

(iv) $\Rightarrow$ (i): As above, if there exist $y \in K$ and $u \in \mathbb{R}^d \setminus \{0\}$ such that $y + \lambda u \in K$ for all $\lambda \in \mathbb{R}$, then $x + \lambda u \in K$ for all $x \in K$ and $\lambda \in \mathbb{R}$. In particular, K has no extreme points, so it has no exposed points.

(ii) $\Leftrightarrow$ (iii): This follows directly from Lemma 2.7.1(ii).

(iii) $\Rightarrow$ (iv): If (iii) holds, then there exists $\alpha \in \mathrm{Int}(\mathrm{rec}(K)^*) \setminus \{0\}$. For a fixed $t \in (m_{K,\alpha}, \infty)$, we know from Proposition 2.7.2 that $K_{\alpha,\, m_{K,\alpha}}$ is a non-empty exposed face of $K^+_{\alpha,t}$, which is d-dimensional, compact and convex. Thus, $K_{\alpha,\, m_{K,\alpha}}$ must itself be compact and convex, so it has at least one extreme point z (Schneider, 2014, Corollary 1.4.4). Now z is necessarily an extreme point of $K^+_{\alpha,t}$, so it follows from Straszewicz's theorem (Schneider, 2014, Theorem 1.4.7) that z is the limit of a sequence of exposed points of $K^+_{\alpha,t}$. But by the convexity of K, every exposed point of $K^+_{\alpha,t}$ must be an exposed point of K, so (iv) holds, as required. $\square$

Using the above results, we now derive necessary and sufficient conditions for a density $f : \mathbb{R}^d \to [0, \infty)$ to belong to the subclass $\mathcal{F}^1$ of log-1-affine densities in $\mathcal{F}_d$.

Proposition 2.7.4. *For $K \in \mathcal{K}$ and $\alpha \in \mathbb{R}^d$, the function $g_{K,\alpha} : \mathbb{R}^d \to [0, \infty)$ defined by $g_{K,\alpha}(x) := \exp(-\alpha^\top x)\mathbb{1}_{\{x \in K\}}$ is integrable if and only if K is line-free and $\alpha \in \mathrm{Int}(\mathrm{rec}(K)^*)$. It follows from this that*

$$\mathcal{F}^1 = \big\{ f_{K,\alpha} := c_{K,\alpha}^{-1}\, g_{K,\alpha} : K \in \mathcal{K},\ K \text{ is line-free and } \alpha \in \mathrm{Int}(\mathrm{rec}(K)^*) \big\}, \tag{2.7.4}$$

where $c_{K,\alpha} := \int_K \exp(-\alpha^\top x)\, dx$.

Proof. The result is clear if $d = 1$, so suppose now that $d \geq 2$. First we consider the case where $\alpha = (\alpha_1, \ldots, \alpha_d) \notin \mathrm{Int}(\mathrm{rec}(K)^*)$, which by Proposition 2.7.3 covers all instances where K is not line-free. By (2.7.2), there exists $u \in \mathrm{rec}(K) \setminus \{0\}$ such that $\alpha^\top u \leq 0$, and we may assume without loss of generality that $u = e_d$. Then for a fixed $x \in \mathrm{Int}\, K$, we can find $\varepsilon > 0$ such that $R_{x,\varepsilon} := \big(\prod_{j=1}^{d-1} [x_j - \varepsilon, x_j + \varepsilon]\big) \times [x_d - \varepsilon, \infty) \subseteq K$. But since $\alpha_d = \alpha^\top e_d \leq 0$, we have

$$c_{K,\alpha} \geq \int_{R_{x,\varepsilon}} \exp(-\alpha^\top w)\, dw = \int_{x_d - \varepsilon}^{\infty} \exp(-\alpha_d w_d)\, dw_d \times \prod_{j=1}^{d-1} \int_{x_j - \varepsilon}^{x_j + \varepsilon} \exp(-\alpha_j w_j)\, dw_j = \infty,$$

so $f_{K,\alpha}$ is not integrable.

Now suppose that K is line-free and $\alpha \in \mathrm{Int}(\mathrm{rec}(K)^*)$. By (2.7.2), the case $\alpha = 0$ is possible if and only if $\mathrm{rec}(K) = \{0\}$. But by Rockafellar (1997, Theorem 8.4), this is equivalent to requiring that K be compact, in which case the result is clear. We can therefore assume that $\alpha \neq 0$. By the final assertion of Proposition 2.7.2(ii), the function $t \mapsto \mu_{d-1}(K_{\alpha,t})^{1/(d-1)}$ is concave and takes strictly positive values on $(m_{K,\alpha}, M_{K,\alpha})$, so there exist $a, b \in \mathbb{R}$ such that $\mu_{d-1}(K_{\alpha,t}) \leq |at + b|^{d-1}$

for all t in this range. By analogy with (2.7.3) and its derivation, we have

$$c_{K,\alpha} = \int_K e^{-\alpha^\top x}\,dx = \|\alpha\|^{-1}\int_{m_{K,\alpha}}^{M_{K,\alpha}} \mu_{d-1}(K_{\alpha,t})\,e^{-t}\,dt \le \|\alpha\|^{-1}\int_{m_{K,\alpha}}^{M_{K,\alpha}} |at+b|^{d-1}e^{-t}\,dt < \infty,$$

as required. The final assertion of the proposition now follows immediately. □

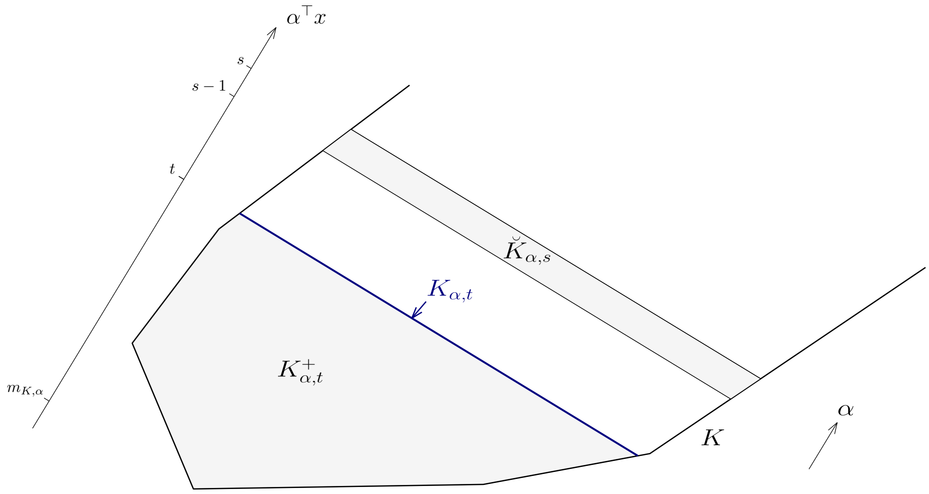

Figure 2.2: Illustration of the sets $K^+_{\alpha,t}$, $K_{\alpha,t}$ and $\breve{K}_{\alpha,s}$.

Now let $\mathcal{F}^1_\star \equiv \mathcal{F}^1_{d,\star}$ denote the collection of all $f_{K,\alpha} \in \mathcal{F}^1$ for which $m_{K,\alpha} = 0$. An immediate consequence of Proposition 2.7.2(ii) and Proposition 2.7.4 is the following:

Corollary 2.7.5. *If $X \sim f \in \mathcal{F}^1$, there exists $x \in \mathbb{R}^d$ such that the density of $X - x$ lies in $\mathcal{F}^1_\star$.*

If $f_{K,\alpha} \in \mathcal{F}^1$, then by Proposition 2.7.2(i) and Proposition 2.7.4, the sets $K^+_{\alpha,t}$ and

$$\breve{K}_{\alpha,t} := K \cap \{x \in \mathbb{R}^d : t-1 \le \alpha^\top x \le t\} \tag{2.7.5}$$

are compact and convex for all $t \in \mathbb{R}$. See Figure 2.2 for an illustration of the sets $K^+_{\alpha,t}$ and $\breve{K}_{\alpha,s}$. We now derive simple bounds on $\mu_d(K^+_{\alpha,t})$ and $\mu_d(\breve{K}_{\alpha,t})$ that apply to all $f_{K,\alpha} \in \mathcal{F}^1_\star$ with $\alpha \neq 0$.

Lemma 2.7.6. *If $f_{K,\alpha} \in \mathcal{F}^1_\star$ and $\alpha \neq 0$, then*

$$\gamma(d,t) := 1 - e^{-t}\sum_{\ell=0}^{d-1}\frac{t^\ell}{\ell!} \le \frac{\mu_d(K^+_{\alpha,t})}{c_{K,\alpha}} \le e^t \tag{2.7.6}$$

for all $t > 0$. Moreover, if $1 \le s \le t-1$, then

$$\mu_d(\breve{K}_{\alpha,t}) \le \frac{t^d - (t-1)^d}{s^d - (s-1)^d}\,\mu_d(\breve{K}_{\alpha,s}). \tag{2.7.7}$$

Proof. The result is clear if $d = 1$, so suppose now that $d \ge 2$. Fix $t > 0$ and observe that, by analogy with (2.7.3), we can write

$$\frac{\mu_d(K^+_{\alpha,t})}{c_{K,\alpha}} = \frac{\int_0^t \mu_{d-1}(K_{\alpha,u})\,du}{\int_0^t \mu_{d-1}(K_{\alpha,u})\,e^{-u}\,du} \times \frac{\int_0^t \mu_{d-1}(K_{\alpha,u})\,e^{-u}\,du}{\int_0^\infty \mu_{d-1}(K_{\alpha,u})\,e^{-u}\,du}. \tag{2.7.8}$$

The first term on the right hand side is bounded above and below by e^t and 1 respectively. The second term is clearly at most 1, and we now show that it is bounded below by $\gamma(d,t)$. This is certainly the case when $t \geq M_{K,\alpha}$, so suppose henceforth that $t < M_{K,\alpha}$. We know from Proposition 2.7.2(ii) that $u \mapsto \mu_{d-1}(K_{\alpha,u})^{1/(d-1)}$ is concave and strictly positive on $(0, M_{K,\alpha})$, so $\mu_{d-1}(K_{\alpha,u}) \geq (u/t)^{d-1}\mu_{d-1}(K_{\alpha,t})$ for all $0 \leq u \leq t$ and $\mu_{d-1}(K_{\alpha,u}) \leq (u/t)^{d-1}\mu_{d-1}(K_{\alpha,t})$ for all $u \geq t$. Therefore, introducing random variables $Y \sim \Gamma(d,1)$ and $W \sim \mathrm{Po}(t)$, we conclude that the second term in (2.7.8) is bounded below by

$$\frac{\int_0^t u^{d-1}\mu_{d-1}(K_{\alpha,t})\,e^{-u}\,du}{\int_0^\infty u^{d-1}\mu_{d-1}(K_{\alpha,t})\,e^{-u}\,du} = \mathbb{P}(Y \leq t) = \mathbb{P}(W \geq d) = \gamma(d,t). \tag{2.7.9}$$

This establishes (2.7.6). Similarly, if $1 \leq s \leq t-1$ and $s < M_{K,\alpha}$, then

$$\frac{\mu_d(\breve{K}_{\alpha,t})}{\mu_d(\breve{K}_{\alpha,s})} = \frac{\int_{t-1}^t \mu_{d-1}(K_{\alpha,u})\,du}{\int_{s-1}^s \mu_{d-1}(K_{\alpha,u})\,du} \leq \frac{\int_{t-1}^t (u/s)^{d-1}\mu_{d-1}(K_{\alpha,s})\,du}{\int_{s-1}^s (u/s)^{d-1}\mu_{d-1}(K_{\alpha,s})\,du} = \frac{t^d - (t-1)^d}{s^d - (s-1)^d}.$$

The bound (2.7.7) holds trivially when $s \geq M_{K,\alpha}$, so we are done. $\square$

Remark. By appealing to Proposition 2.7.2(ii) and stochastic domination arguments, one can in fact show that the reciprocal of the first term on the right hand side of (2.7.8) is bounded below by $dt^{-d}\gamma(d,t)$ and above by $d!\sum_{\ell=1}^{d-1}(-1)^{\ell-1}t^{-\ell}/(d-\ell)!$ (and also that these bounds are tight).

We now turn to the proof of Proposition 2.2.1 in Section 2.2, which makes use of the following two facts from general topology and convex analysis. Recall that $\mathcal{P} \equiv \mathcal{P}_d$ denotes the collection of all polyhedral subsets of $\mathbb{R}^d$, namely those that can be expressed as the intersection of finitely many closed half-spaces (and $\mathbb{R}^d$ itself).

Lemma 2.7.7. *If K is a subset of a topological space E and if $K_1, \ldots, K_\ell \subseteq E$ are closed sets such that $\mathrm{Cl}\,\mathrm{Int}\,K = \bigcup_{j=1}^{\ell} K_j$, then $\mathrm{Cl}\,\mathrm{Int}\,K$ is in fact the union of those K_j for which $\mathrm{Int}\,K_j \neq \emptyset$. Moreover, $\bigcup_{j=1}^{\ell}\mathrm{Int}\,K_j$ is dense in $\mathrm{Cl}\,\mathrm{Int}\,K$.*

Proof of Lemma 2.7.7. We first verify that if $A, B \subseteq E$ and A is closed, then

$$\mathrm{Cl}\,\mathrm{Int}(A \cup B) = (\mathrm{Cl}\,\mathrm{Int}\,A) \cup (\mathrm{Cl}\,\mathrm{Int}\,B) = \mathrm{Cl}\big((\mathrm{Int}\,A) \cup (\mathrm{Int}\,B)\big). \tag{2.7.10}$$

Indeed, recalling that $(\mathrm{Cl}\,P) \cup (\mathrm{Cl}\,Q) = \mathrm{Cl}(P \cup Q)$ and $(\mathrm{Int}\,P) \cup (\mathrm{Int}\,Q) \subseteq \mathrm{Int}(P \cup Q)$ for all $P, Q \subseteq E$, we immediately obtain the second equality and the inclusion $\mathrm{Cl}\,\mathrm{Int}(A \cup B) \supseteq (\mathrm{Cl}\,\mathrm{Int}\,A) \cup (\mathrm{Cl}\,\mathrm{Int}\,B)$. It now remains to show that $\mathrm{Cl}\,\mathrm{Int}(A \cup B) \subseteq (\mathrm{Cl}\,\mathrm{Int}\,A) \cup (\mathrm{Cl}\,\mathrm{Int}\,B)$. To this end, fix $x \in \mathrm{Cl}\,\mathrm{Int}(A \cup B)$ and suppose that $x \notin \mathrm{Cl}\,\mathrm{Int}\,A$, in which case there exists an open neighbourhood U of x that is disjoint from $\mathrm{Int}\,A$. Now let V be an arbitrary open neighbourhood of x and let $W := U \cap V \cap \mathrm{Int}(A \cup B)$. Then $W \subseteq A \cup B$ is a non-empty open set that is disjoint from $\mathrm{Int}\,A$, so $W \not\subseteq A$. Thus, since A is closed by assumption, it follows that $W \cap A^c$ is a non-empty open set contained within B, and hence that $W \cap A^c \subseteq \mathrm{Int}\,B$. We conclude that $V \cap \mathrm{Int}\,B \neq \emptyset$ for all open neighbourhoods V of x, whence $x \in \mathrm{Cl}\,\mathrm{Int}\,B$. This completes the proof of the first equality in (2.7.10).

Moreover, if $K \subseteq E$, then $\mathrm{Cl}\,\mathrm{Int}\,\mathrm{Cl}\,\mathrm{Int}\,K = \mathrm{Cl}\,\mathrm{Int}\,K$; indeed, $\mathrm{Int}\,\mathrm{Cl}\,\mathrm{Int}\,K \supseteq \mathrm{Int}\,\mathrm{Int}\,\mathrm{Int}\,K = \mathrm{Int}\,K$ and $\mathrm{Cl}\,\mathrm{Int}\,\mathrm{Cl}\,\mathrm{Int}\,K \subseteq \mathrm{Cl}\,\mathrm{Cl}\,\mathrm{Cl}\,\mathrm{Int}\,K = \mathrm{Cl}\,\mathrm{Int}\,K$. We deduce from this and (2.7.10) that if $K, K_1, \ldots, K_\ell$ are as in the statement of the lemma, then

$$\mathrm{Cl}\,\mathrm{Int}\,K = \mathrm{Cl}\,\mathrm{Int}\Big(\bigcup_{j=1}^{\ell} K_j\Big) = \mathrm{Cl}\,\Big(\bigcup_{j=1}^{\ell}\mathrm{Int}\,K_j\Big) = \bigcup_{j=1}^{\ell}\mathrm{Cl}\,\mathrm{Int}\,K_j \subseteq \bigcup_{j\,:\,\mathrm{Int}\,K_j \neq \emptyset} K_j.$$

Since $\bigcup_{j\,:\,\mathrm{Int}\,K_j \neq \emptyset} K_j \subseteq \bigcup_{j=1}^{\ell} K_j = \mathrm{Cl}\,\mathrm{Int}\,K$, this yields the first assertion of the lemma. The second assertion follows from the first two equalities in the display above. $\square$

Lemma 2.7.8. *Suppose that $E_1, \ldots, E_\ell \in \mathcal{P}$ have pairwise disjoint interiors and that any intersection $E_r \cap E_s$ with affine dimension $d-1$ is a common face of E_r and E_s. If $P := \bigcup_{s=1}^{\ell} E_s \in \mathcal{P}$, then $E_1, \ldots, E_\ell$ constitutes a polyhedral subdivision of P.*

The proof of Lemma 2.7.8 relies on the auxiliary result below.

Lemma 2.7.9. *Let $d \geq 2$ and let $U \subseteq \mathbb{R}^d$ be a path-connected open set. If we have a finite collection of sets $E_1, \ldots, E_\ell \subseteq \mathbb{R}^d$, each of affine dimension at most $d-2$, then $A := U \setminus \bigcup_{s=1}^{\ell} E_s$ is path-connected. In fact, for any $x, y \in A$, there is a piecewise linear path $\gamma\colon [0,1] \to A$ with $x = \gamma(0)$ and $y = \gamma(1)$.*

Proof of Lemma 2.7.9. Before proving the result in full generality, we first specialise to the case where U is an open ball and proceed by induction on $d \geq 2$. The base case $d = 2$ is trivial, so now consider a general $d > 2$ and fix $x, y \in A$. For each $1 \leq s \leq \ell$, define a linear subspace $W_s := \{z - w : z, w \in \operatorname{aff} E_s\}$ and suppose for the time being that $x - y \notin \bigcup_{s=1}^{\ell} W_s$. Thus, we cannot have $[x, y] \subseteq \operatorname{aff} E_s$ for any s. Consequently, if $\dim(E_s) = d-2$, then $\dim(E_s \cup \{x, y\}) = d-1$, so $H_s := \operatorname{aff}(E_s \cup \{x, y\})$ is the unique affine hyperplane H for which $x, y \in H$ and $E_s \subseteq H$. In other words, if $H \neq H_s$ is any other affine hyperplane through x, y, then $E_s \setminus H \neq \emptyset$, in which case $\operatorname{aff}(E_s \cup H) = \mathbb{R}^d$ and $\dim(H \cap E_s) = \dim(H) + \dim(E_s) - \dim(\mathbb{R}^d) = d-3$. On the other hand, if $\dim(E_s) \leq d-3$, then clearly $\dim(H \cap E_s) \leq \dim(E_s) \leq d-3$ for any affine hyperplane H through x, y. We therefore conclude that there is an affine hyperplane H (of dimension $d-1$) such that $x, y \in H$ and $\dim(H \cap E_s) \leq d-3$ for all s. Since $H \cap U$ is an open ball inside H, it follows by induction that there is a piecewise linear path $\gamma\colon [0,1] \to H$ from x to y, as required.

In general, if x, y are arbitrary points of A, then since A and $\mathbb{R}^d \setminus \bigcup_{s=1}^{\ell} W_s$ have non-empty interior, we can find $z \in A$ such that neither $x - z$ nor $z - y$ lie in $\bigcup_{s=1}^{\ell} W_s$. We have already established that there exist piecewise linear paths in A from x to z and from z to y, so we can concatenate these to obtain a suitable path from x to y. This shows that $U \setminus \bigcup_{s=1}^{\ell} E_s$ is path-connected whenever U is an open ball.

Now let U be an arbitrary path-connected open set. Then for fixed $x, y \in A = U \setminus \bigcup_{s=1}^{\ell} E_s$, there exists a path $\alpha\colon [0,1] \to U$ with $\alpha(0) = x$ and $\alpha(1) = y$. Since U^c is closed and $\operatorname{Im} \alpha$ is compact, there exists $\delta > 0$ such that $B(\alpha(t), \delta) \subseteq U$ for all $t \in [0,1]$. We now claim that there exist $K \in \mathbb{N}$ and $0 \leq t_0, \ldots, t_K \leq 1$ such that $x \in B(\alpha(t_0), \delta)$, $y \in B(\alpha(t_K), \delta)$ and $B(\alpha(t_{j-1}), \delta) \cap B(\alpha(t_j), \delta) \neq \emptyset$ for all $1 \leq j \leq K$. Indeed, by the compactness of $\operatorname{Im} \alpha$, we can extract a finite subset $T \subseteq [0,1]$ such that $\operatorname{Im} \alpha \subseteq \bigcup_{t \in T} B(\alpha(t), \delta)$. Now consider the graph with vertex set T in which $r, s \in T$ are joined by an edge if and only if $B(\alpha(r), \delta) \cap B(\alpha(s), \delta) \neq \emptyset$. If $\emptyset \neq S \subseteq T$ constitutes a connected component of this graph, then $\bigcup_{t \in S} B(\alpha(t), \delta)$ and $\bigcup_{t \in T \setminus S} B(\alpha(t), \delta)$ are disjoint open sets that cover $\operatorname{Im} \alpha$. But since $\operatorname{Im} \alpha$ is connected, it follows that $S = T$ and hence that the graph is connected. Choosing $r, s \in T$ such that $x \in B(\alpha(r), \delta)$ and $y \in B(\alpha(s), \delta)$, we deduce that there is a path in the graph from r to s, as claimed.

Thus, since $\bigcup_{s=1}^{\ell} E_s$ has empty interior, we can find $x_1, x_2, \ldots, x_K \in A$ such that $x_j \in B(\alpha(t_{j-1}), \delta) \cap B(\alpha(t_j), \delta)$ for all $1 \leq j \leq K$. Setting $x_0 := x$ and $x_{K+1} := y$, we have $x_j, x_{j+1} \in B(\alpha(t_j), \delta) \setminus \bigcup_{s=1}^{\ell} E_s$ for $0 \leq j \leq K$, so it follows from the previous argument that there exists a piecewise linear path in A from x_{j-1} to x_j for each j. As before, we can concatenate these to obtain a suitable path from x to y. $\square$

Proof of Lemma 2.7.8. Let $d \geq 2$ and fix $1 \leq r, s \leq \ell$. First we claim that for any fixed $x \in \operatorname{relint}(E_r \cap E_s)$, there exist $r = r_0, r_1, \ldots, r_L = s$ such that $x \in \bigcap_{j=0}^{L} E_{r_j}$ and $E_{r_{j-1}} \cap E_{r_j}$ has affine dimension $d-1$ for all $1 \leq j \leq L$. Indeed, let J be the set of indices $t \in \{1, \ldots, m\}$ such that $x \in E_t$. Since each E_t is closed, we can find $\delta > 0$ such that $B(x, \delta) \cap E_t \neq \emptyset$ if and only if $t \in J$. Now fix

$y \in B(x,\delta) \cap \operatorname{Int} E_r$ and $z \in B(x,\delta) \cap \operatorname{Int} E_s$, and let E' be the union of all sets of the form $E_j \cap E_k$ with affine dimension at most $d-2$, where $j,k \in J$.

By Lemma 2.7.9, there is a piecewise linear path $\gamma\colon [0,1] \to \operatorname{Int} P \cap B(x,\delta) \setminus E'$ with $\gamma(0) = y$ and $\gamma(1) = z$. Let J' be the set of indices $t \in J$ for which $\operatorname{Im}\gamma \cap E_t \neq \emptyset$, and define $\theta(t) := \inf\{u \in [0,1] : \gamma(u) \in E_t\}$ for each $t \in J'$. Now enumerate the elements of J' as $t'_0, t'_1, \ldots, t'_K$ in such a way that $0 = \theta(t'_0) < \theta(t'_1) \leq \theta(t'_2) \leq \ldots \leq \theta(t'_K) < 1$. Then for each $2 \leq J \leq K$, there exists $1 \leq I < J$ such that $\gamma\bigl(\theta(t'_J)\bigr) \in E_{t'_I} \cap E_{t'_J}$, so by the definition of E', it follows that $E_{t'_I} \cap E_{t'_J}$ must have affine dimension $d-1$. Consequently, we can extract a subsequence $r = r_0, r_1, \ldots, r_L = s$ of $t'_0, \ldots, t'_K$ with the required properties.

Setting $E'_j := E_{r_j}$ for $0 \leq j \leq L$, we now show that $E_r \cap E_s = E'_0 \cap E'_L = \bigcap_{j=0}^L E'_j$. Indeed, first note that since $\operatorname{relint}(E'_0 \cap E'_L)$ is a relatively open convex subset of E'_0, it follows from Schneider (2014, Theorem 2.1.2) that there is a unique face F'_0 of E'_0 with $\operatorname{relint}(E'_0 \cap E'_L) \subseteq \operatorname{relint} F'_0$. Moreover, since $E'_0 \cap E'_1$ has affine dimension $d-1$ by construction, the conditions of the lemma imply that $E'_0 \cap E'_1$ is a face of E'_0 that contains x. Thus, $x \in (E'_0 \cap E'_1) \cap \operatorname{relint} F'_0$, and we now appeal to the following consequence of the proof of Schneider (2014, Theorem 2.1.2), which applies to any closed, convex and non-empty $K \subseteq \mathbb{R}^d$: if G, G' are faces of K such that $G \cap \operatorname{relint} G' \neq \emptyset$, then $G \supseteq G'$. Applying this with $K = E'_0$, $G = E'_0 \cap E'_1$ and $G' = F'_0$, and invoking Schneider (2014, Theorem 1.1.15(b)), we deduce that $E'_0 \cap E'_1 \supseteq F'_0 \supseteq E'_0 \cap E'_L$ and hence that $E'_0 \cap E'_L = E'_0 \cap E'_1 \cap E'_L$.

Next, it follows from this and Schneider (2014, Theorem 2.1.2) that there is a face F'_1 of E'_1 with $x \in \operatorname{relint}(E'_0 \cap E'_L) = \operatorname{relint}(E'_0 \cap E'_1 \cap E'_L) \subseteq \operatorname{relint} F'_1$. Since $E'_1 \cap E'_2$ is a face of E'_1 that contains x, we can apply the fact above with $K = E'_1$, $G = E'_1 \cap E'_2$ and $G' = F'_1$ to deduce that $E'_1 \cap E'_2 \supseteq F'_1 \supseteq E'_0 \cap E'_1 \cap E'_L$ and hence that $E'_0 \cap E'_L = E'_0 \cap E'_1 \cap E'_L = E'_0 \cap E'_1 \cap E'_2 \cap E'_L$. Continuing inductively in this vein, we obtain the conclusion that $E_r \cap E_s = E'_0 \cap E'_L = \bigcap_{j=0}^L E'_j$, as claimed.

Now suppose that we have $z \in \bigcap_{j=0}^L E'_j$ and $x, y \in E'_0$ such that $z \in \operatorname{relint}[x,y]$. Then $E'_0 \cap E'_1$ is a face of E'_0 that contains z, so $x, y \in E'_1$. In view of this and the fact that $E'_1 \cap E'_2$ is a face of E'_1 that contains z, it then follows that $x, y \in E'_2$. By repeating this argument, we conclude that $x, y \in \bigcap_{j=0}^L E'_j$. This shows that $E_r \cap E_s$ is a face of $E_r = E'_0$, and it follows by symmetry that $E_r \cap E_s$ is a face of E_s. $\square$

We are now ready to assemble the proof of Proposition 2.2.1. This proceeds via a series of intermediate claims which together imply the result. In Section 2.1.1, we provide only a 'bare-bones' definition of a log-k-affine function $f \in \mathcal{G}_d$ in the sense that the subdomains on which f is log-affine are assumed only to be closed. Starting from this, we show in Claim 1 that f has a 'minimal' representation in which the subdomains are closed, convex sets and the restrictions of f to these sets are distinct log-affine functions. In the remainder of the proof, we investigate the boundary structure of these subdomains more closely and establish that, under the hypotheses of Proposition 2.2.1, these are in fact polyhedral sets that form a subdivision of $\operatorname{supp} f$.

Proof of Proposition 2.2.1. For convenience, we set $g := \log f$. The case $k = 1$ is trivial, so we assume throughout that f is not log-1-affine. By Lemma 2.7.7 and the fact that $K = \operatorname{Cl}\operatorname{Int} K$ for all $K \in \mathcal{K}$ (Schneider, 2014, Theorem 1.1.15(b)), we may assume without loss of generality that there exist $k \geq 2$ closed sets $E'_1, \ldots, E'_k$ with non-empty interiors such that $P := \operatorname{supp} f = \bigcup_{j=1}^k E'_j = \operatorname{Cl}\bigl(\bigcup_{j=1}^k \operatorname{Int} E'_j\bigr)$, and $\theta_1, \ldots, \theta_k \in \mathbb{R}^d$, $\zeta_1, \ldots, \zeta_k \in \mathbb{R}$ such that $g(x) = \theta_j^\top x + \zeta_j$ for all $x \in E'_j$. Moreover, we may suppose that there exist pairwise distinct $\alpha_1, \ldots, \alpha_\ell \in \mathbb{R}^d$ and a subsequence $0 = k_0 < k_1 < \ldots < k_\ell = k$ of the indices $0, 1, \ldots, k$ such that $\theta_j = \alpha_s$ whenever $k_{s-1} < j \leq k_s$. Let $\kappa(f) := \ell$, and for each $1 \leq s \leq \ell$, let $E_s := \bigcup_{j=k_{s-1}+1}^{k_s} E'_j$.

Claim 1. *$E_1, \ldots, E_\ell$ are closed, convex sets with pairwise disjoint and non-empty interiors. Moreover, if $\theta_i = \theta_j$, then $\zeta_i = \zeta_j$, i.e. there exist $\beta_1, \ldots, \beta_\ell \in \mathbb{R}$ such that $g(s) = g_s(x) := \alpha_s^\top x + \beta_s$ for all $x \in E_s$. Thus, the restrictions of g to the sets $E_1, \ldots, E_\ell$ are distinct affine functions $g_1, \ldots, g_\ell$.*

Proof of Claim 1. If $E \subseteq \mathbb{R}^d$ has non-empty interior and $g_1, g_2 \colon E \to \mathbb{R}$ are affine functions that agree on a non-empty open subset of E, then g_1, g_2 must in fact agree everywhere on E, so $(\operatorname{Int} E_r) \cap (\operatorname{Int} E_s) = \emptyset$ whenever $r \neq s$. Moreover, for distinct $i, j \in \{k_{s-1}+1, \ldots, k_s\}$, fix $x_i' \in \operatorname{Int} E_i'$ and $x_j' \in \operatorname{Int} E_j'$, so that $g(x) = \alpha_s^\top x + \zeta_j$ for all $x \in [x_i', x_j']$ sufficiently close to x_j' and $g(x) = \alpha_s^\top x + \zeta_i$ for all $x \in [x_i', x_j']$ sufficiently close to x_i'. But since g is concave on $[x_i', x_j']$, it follows that $\zeta_i = \zeta_j$, as required. Thus, there exist $\beta_1, \ldots, \beta_\ell \in \mathbb{R}$ such that $g(x) = g_s(x) := \alpha_s^\top x + \beta_s$ for all $x \in E_s$.

It remains to show that each E_s is convex. Fix $y \in \operatorname{Int} E_s$ and suppose for a contradiction that $(\operatorname{conv} E_s) \setminus E_s$ is non-empty. Since $\operatorname{conv} E_s \subseteq \operatorname{Cl}(\operatorname{conv} E_s) = \operatorname{Cl}\operatorname{Int}(\operatorname{conv} E_s)$, it follows that $\operatorname{Int}(\operatorname{conv} E_s) \setminus E_s \subseteq P$ is a non-empty open set. We know from Lemma 2.7.7 that $\bigcup_{r=1}^{\ell} \operatorname{Int} E_r$ is dense in P, i.e. that it has non-empty intersection with any non-empty open subset of P. Thus, there exist $r \neq s$ such that $W := (\operatorname{Int} E_r) \cap \operatorname{Int}(\operatorname{conv} E_s) \setminus E_s$ is a non-empty open set. Now for each $x \in W$, there exist $x_1, x_2 \in E_s$ such that $x \in [x_1, x_2]$. Since g is concave on $[x_1, x_2]$ and $g(x_j) = \alpha_s^\top x_j + \beta_s$ for $j = 1, 2$, we have $g(x) \geq \alpha_s^\top x + \beta_s$. On the other hand, since g is concave on $[x, y]$ and $g(z) = \alpha_s^\top z + \beta_s$ for all $z \in [x, y]$ sufficiently close to y, it follows that $g(x) \leq \alpha_s^\top x + \beta_s$. Thus, $g(x) = \alpha_s^\top x + \beta_s = \alpha_r^\top x + \beta_r$ for all $x \in W \subseteq \operatorname{Int} E_r$, so $\alpha_r = \alpha_s$ and $\beta_r = \beta_s$. This contradicts the fact that $\alpha_1, \ldots, \alpha_\ell$ are pairwise distinct, so the proof of the claim is complete. □

Claim 2. *If $E_r \cap E_s \neq \emptyset$ and $r \neq s$, then $E_r \cap E_s$ is a closed, convex subset of ∂E_r. Moreover, if $E_r \cap E_s$ has affine dimension $d-1$, then there exists a unique closed half-space H_{rs}^+ containing E_r such that $E_r \cap E_s = E_r \cap H_{rs}$, where $H_{rs} := \partial H_{rs}^+$. Thus, in this case, $E_r \cap E_s$ is a common (exposed) facet of E_r and E_s, and we must have $H_{sr}^+ = (\operatorname{Int} H_{rs}^+)^c$ and $H_{rs} = H_{sr}$.*

Proof of Claim 2. Since E_s is convex and $\operatorname{Int} E_s \subseteq (\operatorname{Int} E_r)^c$, we have $E_s = \operatorname{Cl}\operatorname{Int} E_s \subseteq (\operatorname{Int} E_r)^c$, so $E_r \cap E_s$ is a closed, convex subset of ∂E_r. Then by Schneider (2014, Theorem 2.1.2), there exists a unique proper face F of E_r (whose affine dimension is at most $d-1$) such that $\operatorname{relint}(E_r \cap E_s) \subseteq \operatorname{relint} F$. Now suppose that $E_r \cap E_s$ has affine dimension $d-1$. Then F is a facet of E_r, so by Schneider (2014, Theorem 2.1.2) and the final observation in the paragraph after the proof of this result (Schneider, 2014, page 75), there exists a closed half-space $H_{rs}^+ \supseteq E_r$ such that $H_{rs} := \partial H_{rs}^+$ is a supporting hyperplane to E_r with $F = E_r \cap H_{rs}$. Note that a closed half-space H_{rs}^+ with these properties must be unique. Furthermore, since the affine functions g_r and g_s agree on a relatively open subset of H_{rs}, namely $\operatorname{relint}(E_r \cap E_s)$, they must agree everywhere on H_{rs}.

We now show that $E_r \cap E_s = F$. If this is not the case, then there exist $y \in F \setminus (E_r \cap E_s)$ and $z \in \operatorname{relint}(E_r \cap E_s) \subseteq \operatorname{relint} F$. Thus, there is some $x \in (y, z]$ that belongs to $\partial(E_r \cap E_s) \cap (\operatorname{relint} F)$ and there exists $\eta > 0$ such that $B(x, \eta) \cap H_{rs} \subseteq F \subseteq E_r$. Now fix $w \in \operatorname{Int} E_r$ and observe that we can find $\delta \in (0, \eta)$ such that $E_s \not\subseteq B(x, \delta)$ and $B(x, \delta) \cap H_{rs}^+ \subseteq \operatorname{conv}(\{w\} \cup B(x, \eta) \cap H_{rs}) \subseteq E_r$. Since $E_r \subseteq H_{rs}^+$, it follows that $B(x, \delta) \cap H_{rs}^+ = B(x, \delta) \cap E_r$. Writing $H_{sr}^+ := (\operatorname{Int} H_{rs}^+)^c$ for the other closed half-space bounded by H_{rs}, we note in addition that $E_s \subseteq H_{sr}^+$; indeed, if there did exist $\tilde{x} \in E_s \setminus H_{sr}^+ = E_s \cap \operatorname{Int} H_{rs}^+$, then $[x, \tilde{x}]$ would be contained within E_s and also have non-empty intersection with $B(x, \delta) \cap \operatorname{Int} H_{rs}^+ = \operatorname{Int}(B(x, \delta) \cap H_{rs}^+) \subseteq \operatorname{Int} E_r$, which would contradict the fact that $E_s = \operatorname{Cl}\operatorname{Int} E_s \subseteq (\operatorname{Int} E_r)^c$.

Next, fix $x' \in E_s \setminus B(x, \delta) \subseteq H_{sr}^+ \setminus B(x, \delta)$ and note that there exists $\delta' \in (0, \delta]$ such that for every $y' \in B(x, \delta') \cap \operatorname{Int} H_{sr}^+$, we can find $z' \in B(x, \eta) \cap H_{rs} \subseteq F \subseteq H_{rs}$ with $y' \in [x', z']$. Thus, if y', z' are as above, then since $g(x') = g_s(x')$ and $g(z') = g_r(z') = g_s(z')$, it follows from the concavity of g on $[x', z']$ that $g(y') \geq g_s(y')$. On the other hand, there exists $w' \in [x, x'] \subseteq E_s$ sufficiently close to x such that $w' \in [y', z'']$ for some $z'' \in B(x, \eta) \cap H_{rs} \subseteq F \subseteq H_{rs}$. As before, we have

$g(w') = g_s(w')$ and $g(z'') = g_r(z'') = g_s(z'')$, so $g(y') \leq g_s(y')$ by the concavity of g on $[w', z'']$. We therefore conclude that $g(y') = g_s(y')$ for all $y' \in B(x, \delta') \cap \operatorname{Int} H_{sr}^+$. Note that we cannot have $B(x, \delta') \cap \operatorname{Int} H_{sr}^+ \subseteq \operatorname{Int} E_s$; indeed, it would follow that $B(x, \delta') \cap H_{rs} \subseteq E_r \cap (\operatorname{Cl} \operatorname{Int} E_s) = E_r \cap E_s$, and since $\operatorname{aff}(E_r \cap E_s) = H_{rs}$, this would contradict the fact that $x \in \partial(E_r \cap E_s)$. Thus, there exists $t \neq r, s$ such that the intersection of $\operatorname{Int} E_t$ with $B(x, \delta') \cap \operatorname{Int} H_{sr}^+$ is a non-empty open set, which we denote by U. We see that the affine functions g_s and g_t both agree with g on U, so in fact $g_s = g_t$ on $\mathbb{R}^d$. This contradicts Claim 1, so it must therefore be the case that $E_r \cap E_s = F = E_r \cap H_{rs}$, as required.

By interchanging E_r and E_s in the argument above, we deduce that there exists a closed half-space H^+ containing E_s such that $E_r \cap E_s = E_s \cap \partial H^+$. Then $E_r \cap E_s \subseteq H_{rs} \cap \partial H^+ \subseteq H_{rs}$, so $\dim(E_r \cap E_s) = \dim(H_{rs} \cap \partial H^+) = \dim(H_{rs}) = d - 1$. It follows that $\partial H^+ = H_{rs}$ and hence that $H^+ = H_{sr}^+$, which yields the final assertion of the claim. □

Since $P \in \mathcal{P}$ by hypothesis, there exist closed half-spaces $H_1^+, \ldots, H_M^+$ such that $P = \bigcap_{j=1}^M H_j^+$. For each $1 \leq j \leq M$, let $H_j := \partial H_j^+$, and for each $1 \leq r \leq \ell$, let I_r be the set of indices $s \in \{1, \ldots, \ell\}$ for which $E_r \cap E_s$ has affine dimension $d - 1$.

Claim 3. *If $1 \leq r \leq \ell$ and $x \in \partial E_r$, then either $x \in E_r \cap H_j$ for some $1 \leq j \leq M$ or $x \in E_r \cap E_s = E_r \cap H_{rs}$ for some $s \in I_r$.*

Proof of Claim 3. Fix $1 \leq \ell \leq r$, and note that $\partial P \subseteq \bigcup_{j=1}^M H_j$ and $\operatorname{Cl} E_r^c \subseteq \operatorname{Cl}\left(P^c \cup \bigcup_{s \neq r} E_s\right) = (\operatorname{Cl} P^c) \cup \left(\bigcup_{s \neq r} E_s\right) = P^c \cup (\partial P) \cup \left(\bigcup_{s \neq r} E_s\right)$. Since $\operatorname{Int} E_r \cap \partial P \subseteq \operatorname{Int} P \cap \partial P = \emptyset$, we have $E_r \cap \partial P \subseteq \partial E_r$. Recalling from Claim 2 that $\bigcup_{s \neq r} (E_r \cap E_s) \subseteq \partial E_r$, we deduce that $\partial E_r = E_r \cap \operatorname{Cl} E_r^c$ is the union of the sets $E_r \cap H_1, \ldots, E_r \cap H_M$ and $\bigcup_{s \neq r} (E_r \cap E_s)$, all of which are closed. In view of Claim 2 and Lemma 2.7.7, in which we set $E := \partial E_r$ (equipped with the subspace topology), it suffices to show that $E_r \cap E_s$ has non-empty interior in ∂E_r if and only if $s \in I_r$.

Suppose first that $s \in I_r$, so that $\dim(E_r \cap E_s) = d - 1$. Then $E_r \cap E_s = E_r \cap H_{rs} \subseteq \partial E_r$ and $\operatorname{aff}(E_r \cap E_s) = H_{rs}$ by Claim 2, so for a fixed $x \in \operatorname{relint}(E_r \cap E_s)$, there exists $\delta > 0$ such that $B(x, \delta) \cap H_{rs} \subseteq E_r \cap E_s$. Now fix $w \in \operatorname{Int} E_r$ and note that there exists $\delta' \in (0, \delta]$ such that $B(x, \delta') \cap H_{rs}^+ \subseteq \operatorname{conv}(\{w\} \cup B(x, \delta) \cap H_{rs}) \subseteq E_r$. Since $B(x, \delta') \cap \operatorname{Int} H_{sr}^+ \subseteq E_r^c$ and $B(x, \delta') \cap \operatorname{Int} H_{rs}^+ = \operatorname{Int}(B(x, \delta) \cap H_{rs}^+) \subseteq \operatorname{Int} E_r$, we deduce that $B(x, \delta') \setminus H_{rs} = \emptyset$ and hence that $B(x, \delta') \cap \partial E_r = (B(x, \delta') \cap H_{rs}) \cap \partial E_r \subseteq E_r \cap E_s$. Thus, $E_r \cap E_s$ has non-empty interior in $E = \partial E_r$, as required.

On the other hand, if $s \notin I_r$, then $F := E_r \cap E_s$ has affine dimension at most $d - 2$. Fix $x \in F$ and $w \in \operatorname{Int} E_r$, and let $\eta > 0$ be such that $B(w, \eta) \subseteq \operatorname{Int} E_r$. Then there exist $w_1, w_2 \in B(w, \eta)$ such that $w_1 \notin \operatorname{aff} F$ and $w_2 \notin \operatorname{aff}(F \cup \{w_1\})$. Now let $A := \operatorname{aff}\{x, w_1, w_2\}$. Then $A \cap F = \{x\}$ and $A \cap B(w, \eta) \neq \emptyset$ by construction, so $A \cap E_r$ is a closed, convex set with $\dim(A \cap E_r) = 2$.

We now verify that $\partial(A \cap E_r) = A \cap \partial E_r$. Indeed, since $A \cap \operatorname{Int} E_r$ and $\partial(A \cap E_r)$ are disjoint, we have $\partial(A \cap E_r) \subseteq A \cap \partial E_r$. For the reverse inclusion, note that if $x \in A \cap \partial E_r$, then there exists an open half-space $H^- \subseteq \mathbb{R}^d$ such that $H^- \cap E_r = \emptyset$ and ∂H^- is a supporting hyperplane to E_r at x. Since $A \cap \operatorname{Int} E_r \neq \emptyset$, we cannot have $A \subseteq \partial H^-$, so $\dim(A \cap \partial H^-) = 1$ and therefore $x \in \operatorname{Cl}(A \cap H^-) \subseteq \operatorname{Cl}(A \setminus E_r) \subseteq (\operatorname{relint}(A \cap E_r))^c$, as required.

Since $x \in F \subseteq A \cap \partial E_r = \partial(A \cap E_r)$, it follows that $x \in \operatorname{Cl}(\partial(A \cap E_r) \setminus \{x\})$. By combining the observations above, we see that $\partial(A \cap E_r) \setminus \{x\} = (A \setminus \{x\}) \cap \partial E_r \subseteq F^c \cap \partial E_r$, so $x \in \operatorname{Cl}(F^c \cap \partial E_r)$. Since $x \in F$ was arbitrary, we conclude that $F \subseteq \operatorname{Cl}(F^c \cap \partial E_r)$, which implies that $F = E_r \cap E_s$ has non-empty interior in ∂E_r. □

Claim 4. *For each $1 \leq r \leq \ell$, we have $E_r = P \cap \bigcap_{s \in I_r} H_{rs}^+$, so in particular $E_r \in \mathcal{P}$.*

Proof of Claim 4. For a fixed $1 \leq r \leq \ell$, we already know that $E_r \subseteq P \cap \bigcap_{s \in I_r} H_{rs}^+$. Now fix $x \in E_r^c$ and $w \in \operatorname{Int} E_r$, and note that there exists $y \in \partial E_r \cap [x, w)$. By Claims 2 and 3, there is a closed half-space $H^+ \supseteq E_r$ with $y \in \partial H^+$ such that either $H^+ = H_j^+$ for some $1 \leq j \leq M$, or $H^+ = H_{rs}^+$ for some $s \in I_r$. In all cases, we have $w \in H^+$, so it follows that $x \notin H^+$ and hence that $x \notin P \cap \bigcap_{s \in I_r} H_{rs}^+$. □

We have now established the first part of Proposition 2.2.1, as well as the fact that $E_r \cap E_s$ is a common face of E_r and E_s whenever this intersection has affine dimension $d-1$. In view of Claim 1, a direct application of Lemma 2.7.8 yields the conclusion that $E_1, \ldots, E_\ell$ constitutes a polyhedral subdivision of P. Since $|I_r| \leq k-1$ for all $1 \leq r \leq \ell$, it follows from Claim 4 that each E_r can be expressed as the intersection of at most $M + |I_r| \leq M + k - 1$ closed half-spaces. In view of Bruns and Gubeladze (2009, Theorem 1.6), this implies the last assertion of Proposition 2.2.1.

Finally, to show that the triples $(\alpha_j, \beta_j, E_j)_{j=1}^{\kappa(f)}$ are unique up to reordering, we make the following observation: if g is affine on some $\tilde{E} \in \mathcal{K}$ with $\tilde{E} \subseteq P$, then there exists a unique $1 \leq r \leq \ell$ such that $\tilde{E}_j \subseteq E_r$. Indeed, it cannot happen that there exist distinct $1 \leq r, s \leq \ell$ such that $\operatorname{Int} \tilde{E}$ intersects both $\operatorname{Int} E_r$ and $\operatorname{Int} E_s$, since $g_1, \ldots, g_\ell$ are distinct affine functions by Claim 1. Thus, there exists a unique $1 \leq r \leq \ell$ such that $\operatorname{Int} \tilde{E} \subseteq \operatorname{Int} E_r$, so $\tilde{E} = \operatorname{Cl} \operatorname{Int} \tilde{E} \subseteq \operatorname{Cl} \operatorname{Int} E_r = E_r$, whereas for $s \neq r$, we cannot have $\tilde{E} \subseteq E_s$ since $\operatorname{Int} \tilde{E} \not\subseteq \operatorname{Int} E_s$.

Consequently, if $\tilde{E}_1, \ldots, \tilde{E}_{\ell'} \in \mathcal{K}$ are such that $P = \bigcup_{j=1}^{\ell'} \tilde{E}_j$ and the restrictions of g to these sets are distinct affine functions, then the observation above implies that $\ell' = \ell$ and that there is some permutation $\pi \colon \{1, \ldots, \ell\} \to \{1, \ldots, \ell\}$ such that $\tilde{E}_{\pi(j)} \subseteq E_j$ for all $1 \leq j \leq \ell$. In fact, we must have $\tilde{E}_{\pi(j)} = E_j$ for all j. Indeed, if $E_j \setminus \tilde{E}_{\pi(j)} \neq \emptyset$ for some j, then since $E_j = \operatorname{Cl} \operatorname{Int} E_j$, it would follow that $W := (\operatorname{Int} E_j) \setminus \tilde{E}_{\pi(j)}$ is a non-empty open subset of P. Since $\tilde{E}_{\pi(j)} \cap W = \emptyset$ and $\tilde{E}_{\pi(j')} \cap W \subseteq E_{j'} \cap \operatorname{Int} E_j = \emptyset$ for all $j' \neq j$, this would imply that $\bigcup_{j=1}^{\ell'} \tilde{E}_j \subseteq P \setminus W \subsetneq P$. This contradiction completes the proof. □

Now for $k \in \mathbb{N}$ and $P \in \mathcal{P} \equiv \mathcal{P}_d$, denote by $\mathcal{F}^k(P) \equiv \mathcal{F}_d^k(P)$ the collection of all $f \in \mathcal{F}_d$ for which $\kappa(f) \leq k$ and $\operatorname{supp} f = P$. For $m \in \mathbb{N}_0$, recall that $\mathcal{P}^m \equiv \mathcal{P}_d^m$ denotes the collection of all $P \in \mathcal{P}_d$ with at most m facets (and that we view $\mathbb{R}^d$ as a polyhedral set with 0 facets). Finally, for $k \in \mathbb{N}$ and $m \in \mathbb{N}_0$, define $\mathcal{F}^k(\mathcal{P}^m) \equiv \mathcal{F}_d^k(\mathcal{P}_d^m) := \bigcup_{P \in \mathcal{P}^m} \mathcal{F}^k(P)$.

Proposition 2.7.10. *For $k \in \mathbb{N}$ and $m \in \mathbb{N}_0$, the subclass $\mathcal{F}^k(\mathcal{P}^m)$ is non-empty if and only if $k + m \geq d + 1$.*

For one direction of the proof, we require the following basic result:

Lemma 2.7.11. *Every line-free $P \in \mathcal{P}_d$ has at least d facets. Moreover, every bounded $P \in \mathcal{P}_d$ (i.e. every d-dimensional polytope) has at least $d+1$ facets.*

Proof of Lemma 2.7.11. Fix $P \in \mathcal{P}$ and consider any representation of P as the intersection of finitely many closed half-spaces $H_1^+, \ldots, H_m^+$, where $H_j^+ = \{x \in \mathbb{R}^d : \alpha_j^\top x \leq b_j\}$ for some $\alpha_j \in \mathbb{R}^d \setminus \{0\}$ and $b_j \in \mathbb{R}$. Then $C := \bigl\{\sum_{j=1}^m \lambda_j \alpha_j : \lambda_j \geq 0 \text{ for all } j\bigr\}$ is a closed, convex cone, and note that $\operatorname{rec}(P) = \{u \in \mathbb{R}^d : \alpha_j^\top u \leq 0 \text{ for all } j\} = -C^*$. Thus, if P is line-free, then $\operatorname{Int}(\operatorname{rec}(P)^*) = -\operatorname{Int} C$ is non-empty by Proposition 2.7.3, so $m \geq \dim(C) = d$. On the other hand, if P is bounded, then $\operatorname{rec}(P) = -C^* = \{0\}$ by Rockafellar (1997, Theorem 8.4), so $C = \mathbb{R}^d$. As above, this implies that $m \geq \dim(C) = d$, and observe that we cannot have $m = \dim(C) = d$, since then $\alpha_1, \ldots, \alpha_d$ would be linearly independent, in which case $C \neq \mathbb{R}^d$. This implies that $m \geq d+1$, as required. In both the line-free and bounded cases, the result follows on applying Bruns and Gubeladze (2009, Theorem 1.6). □

Proof of Proposition 2.7.10. Suppose first that $k \in \mathbb{N}$ and $m \in \mathbb{N}_0$ are such that $\mathcal{F}^k(\mathcal{P}^m)$ is non-empty. Then for $f \in \mathcal{F}^k(\mathcal{P}^m)$, we deduce from the final assertion of Proposition 2.2.1 that there are polyhedral sets $E_1, \ldots, E_{\kappa(f)} \in \mathcal{P}^{k+m-1}$ such that $f|_{E_j}$ is log-1-affine and integrable for each $1 \leq j \leq \kappa(f)$. Thus, by Proposition 2.7.4 and Lemma 2.7.11, each E_j is line-free and therefore has at least d facets. It follows that $k + m - 1 \geq d$, as desired.

To establish the converse, note that since the classes $\mathcal{F}^k(\mathcal{P}^m)$ are nested in k and m by definition, it will suffice to consider each $k \in \{1, \ldots, d+1\}$ in turn and exhibit a density $f_{k,\,d+1-k}$ on $\mathbb{R}^d$ that lies in $\mathcal{F}^k(\mathcal{P}^{d+1-k}) \equiv \mathcal{F}_d^k(\mathcal{P}_d^{d+1-k})$. We proceed by induction on $d \in \mathbb{N}$. When $d = 1$, the univariate densities $f_{1,1} \colon x \mapsto e^{-x}\,\mathbb{1}_{\{x \geq 0\}}$ and $f_{2,0} \colon x \mapsto e^{-|x|}/2$ have the required properties. For a general $d \geq 2$, first fix $k \in \{1, \ldots, d\}$ and define $f_{k,\,d+1-k} \colon \mathbb{R}^d \to [0, \infty)$ by

$$f_{k,\,d+1-k}(x_1, \ldots, x_d) := f_{k,\,d-k}(x_1, \ldots, x_{d-1})\, e^{-x_d}\, \mathbb{1}_{\{x_d \geq 0\}},$$

where $f_{k,\,d-k} \colon \mathbb{R}^{d-1} \to [0, \infty)$ is an element of $\mathcal{F}_{d-1}^k(\mathcal{P}_{d-1}^{d-k})$ whose existence is guaranteed by the inductive hypothesis. Then $\int_{\mathbb{R}^d} f_{k,\,d+1-k} = \bigl(\int_{\mathbb{R}^{d-1}} f_{k,\,d-k}\bigr)\bigl(\int_0^\infty e^{-x_d}\,dx_d\bigr) = 1$ by Fubini's theorem, so $f_{k,\,d+1-k}$ is a density, which is easily seen to lie in $\mathcal{F}_d$. Observe also that $\operatorname{supp} f_{k,\,d+1-k} = (\operatorname{supp} f_{k,\,d-k}) \times [0, \infty) \in \mathcal{P}_d^{d+1-k}$; indeed, $P := \operatorname{supp} f_{k,\,d-k}$ has (at most) $d - k$ facets by induction, and we see that F is a facet of $\operatorname{supp} f_{k,\,d+1-k} = P \times [0, \infty)$ if and only if either $F = P \times \{0\}$ or $F = F' \times [0, \infty)$ for some facet F' of P. Furthermore, since $f_{k,\,d-k} \in \mathcal{F}_{d-1}^k(\mathcal{P}_{d-1}^{d-k})$, there are closed sets $E_1', \ldots, E_k' \subseteq \mathbb{R}^{d-1}$ such that $P = \operatorname{supp} f_{k,\,d-k} = \bigcup_{j=1}^k E_j'$ and $\log f_{k,\,d-k}$ is affine on each E_j'. It follows that $\log f_{k,\,d+1-k}$ is affine on each of the sets $E_1' \times [0, \infty), \ldots, E_k' \times [0, \infty)$, whose union is $P \times [0, \infty) = \operatorname{supp} f_{k,\,d+1-k}$. This shows that $f_{k,\,d+1-k} \in \mathcal{F}_d^k(\mathcal{P}_d^{d+1-k})$.

Finally, to define $f_{d+1,\,0}$, we fix $u_1, \ldots, u_{d+1} \in \mathbb{R}^d$ such that $S := \operatorname{conv}\{u_1, \ldots, u_{d+1}\}$ is a d-simplex with $0 \in \operatorname{Int} S$. Then as remarked at the start of Section 2.7, the Minkowski functional $\rho_S \colon w \mapsto \inf\{\lambda > 0 : w \in \lambda S\} \in [0, \infty)$ is a convex (and therefore continuous) function on $\mathbb{R}^d$, and by Xu and Samworth (2021, Proposition 2), there exists $c > 0$ such that $f_{d+1,\,0} \colon x \mapsto ce^{-\rho_S(x)}$ is a density in $\mathcal{F}_d$. Defining $F_j := \operatorname{conv}\{u_1, \ldots, u_{j-1}, u_{j+1}, \ldots, u_{d+1}\}$ for $1 \leq j \leq d+1$, we see that the facets of S are precisely $F_1, \ldots, F_{d+1}$, and hence that $\log f_{d+1,\,0} = \log c - \rho_S$ is affine on $C_j := \bigcup_{\lambda \in [0,\infty)} \lambda F_j$ for each $1 \leq j \leq d+1$. Since $\operatorname{supp} f_{d+1,\,0} = \mathbb{R}^d = \bigcup_{\lambda \in [0,\infty)} \lambda S = \bigcup_{j=1}^{d+1} C_j$, it follows that $f_{d+1,\,0} \in \mathcal{F}_d^{d+1}(\mathcal{P}_d^0)$, as required. □

To conclude this subsection, we also record the fact that if $d \leq 3$, then every polytope in $\mathcal{P}^m \equiv \mathcal{P}_d^m$ can be triangulated into $O(m)$ simplices.

Lemma 2.7.12. *If $d \leq 3$ and $P \in \mathcal{P}^m$ is a polytope, then P has at most $2m$ vertices and there is a triangulation of P that contains at most $6m$ simplices.*

Proof. The cases $d = 1, 2$ are trivial, so suppose now that $d = 3$. If P has v vertices, e edges and f facets, then Euler's formula asserts that $v - e + f = 2$ (e.g. Kalai, 2004, Section 20.1). The edges of P induce a graph structure on the set of vertices of P, and it is easy to see that the degree of every vertex is at least 3. This implies that $2e \geq 3v$, and we deduce from Euler's formula that $v \leq 2(f - 2)$. The result above follows from the fact that P has a triangulation that contains at most $3v - 11$ simplices (Edelsbrunner et al., 1990). □

Remark. In the case $d = 3$, we also have the bound $2e \geq 3f$, since every face has at least 3 edges and every edge belong to exactly 2 faces. It then follows from Euler's formula that $f \leq 2(v - 2)$.

In addition, when $d = 2$, we have the following useful result about polyhedral subdivisions.

Lemma 2.7.13. *If $d = 2$ and $E_1, \ldots, E_k$ is a subdivision of a polyhedral set $P \in \mathcal{P}^m$, then $\sum_{j=1}^k |\mathcal{F}(E_j)| \lesssim k + m$.*

Proof. Regardless of whether or not P is bounded, observe that P^c can be subdivided into m polyhedral sets in such a way that the intersection of each of these sets with P is a facet of P. It

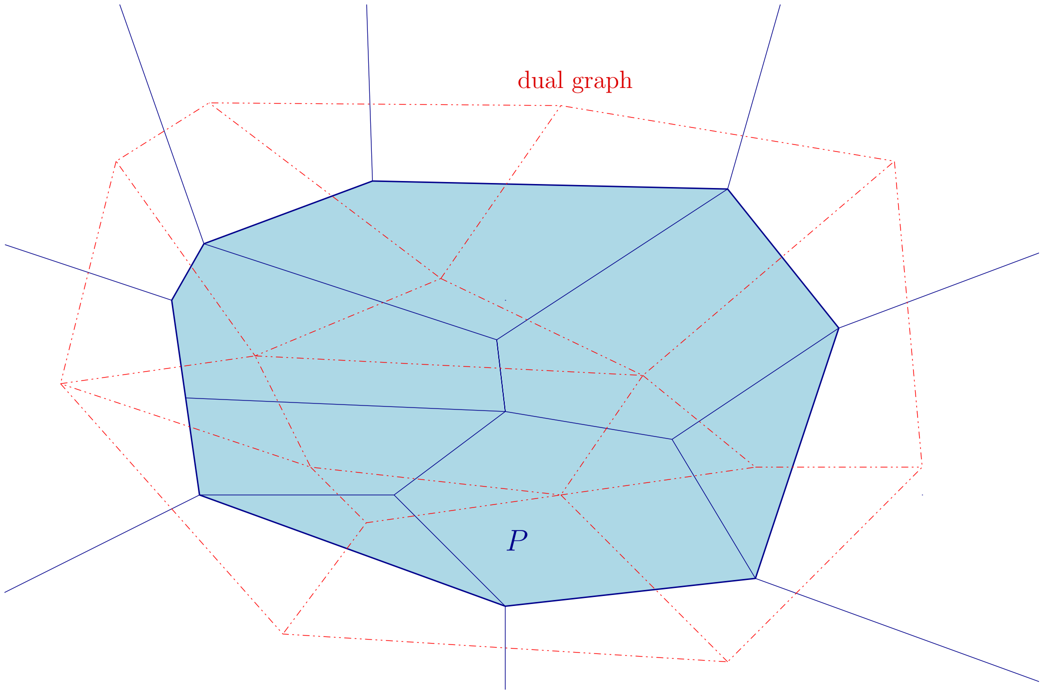

Figure 2.3: Illustration of the configuration in Lemma 2.7.13.

may be helpful to refer to Figure 2.3, in which P is represented by the blue shaded region and the subdivisions of P and P^c are indicated by the blue lines.

Having dissected $\mathbb{R}^2 = P \cup P^c$ into $k+m$ polyhedral regions, we now form the *dual graph* G' of this configuration by fixing a point in each region and joining two points by an edge if the corresponding regions share a (non-trivial) line segment. This is highlighted in red in Figure 2.3. In this graph, the degree of the vertex inside E_j is simply the number of facets of E_j, and the sum of the degrees of all $k+m$ vertices is equal to twice the number of edges of G'. But G' is *planar* (i.e. it can be drawn in the plane in such a way that no two edges cross), so it has at most $3(k+m)-6$ edges (Kalai, 2004, Section 20.1). Together with the previous observations, this implies the desired result. □

2.7.2 Auxiliary results for bracketing entropy calculations

The results in this subsection hold for any $d \in \mathbb{N}$. First, we consider log-concave functions f_0, f whose restrictions to some $K \in \mathcal{K}^b$ are close in Hellinger distance, and obtain pointwise bounds on f under the assumption that f_0 is bounded away from 0 on K. Henceforth, we write $f_K := f_{K,0} = \mu_d(K)^{-1}\mathbb{1}_K \in \mathcal{F}^1$ for the uniform density on K.

Recall that $\Phi \equiv \Phi_d$ denotes the set of all upper semi-continuous, concave functions $\phi\colon \mathbb{R}^d \to [-\infty,\infty)$, and that $\mathcal{G} \equiv \mathcal{G}_d = \{e^\phi : \phi \in \Phi\}$. For $\phi \in \Phi$ and $x \in \mathbb{R}^d$, let $D_{\phi,x} := \{w \in \mathbb{R}^d : \phi(w) > \phi(x)\}$.

Lemma 2.7.14. *Fix $K \in \mathcal{K}^b$ and $f_0 \in \mathcal{F}$, and suppose that there exists $\theta \in [1,\infty)$ such that $f_0 \geq \theta^{-1} f_K$ on K. Let $f \in \mathcal{G}$ and $\delta > 0$ be such that $\int_K \bigl(\sqrt{f} - \sqrt{f_0}\bigr)^2 \leq \delta^2$. Then setting $\phi := \log f \in \Phi$, we have the following:*

(i) If $x \in K$ satisfies $\mu_d(K \setminus D_{\phi,x}) \geq 4\delta^2\theta\mu_d(K)$, then
$\phi(x) + \log \mu_d(K) \geq -4\delta\{\theta\mu_d(K)/\mu_d(K \setminus D_{\phi,x})\}^{1/2} - \log\theta$.

(ii) If $\theta = 1$ and $\delta \in (0, 2^{-3/2}]$, then $f_0 = f_K$ and $\phi + \log\mu_d(K) \leq (8\sqrt{2}d)\delta$ on K.

(iii) There exist $s_d \geq 1$, depending only on d, and a universal constant $s' > 0$ such that if $\theta > 1$ and $\delta \in (0, (8\theta)^{-1/2}]$, then $\phi + \log \mu_d(K) \leq \log\bigl(s_d \log^d(e\theta) - s_d + 1\bigr) + s'(d^{(d+1)}\delta)^{2/(d+2)}$ on K.

Proof. For (i), we may assume that $\phi(x) + \log \mu_d(K) < -\log\theta$, for otherwise there is nothing to prove. Setting $c := \theta\mu_d(K)$, we have $e^{\phi(w)/2} \leq e^{\phi(x)/2} < c^{-1/2} \leq \sqrt{f_0(w)}$ for all $w \in K \setminus D_{\phi,x}$, so

$$\delta^2 \geq \int_{K\setminus D_{\phi,x}} \bigl(\sqrt{f_0} - e^{\phi/2}\bigr)^2 \geq \int_{K\setminus D_{\phi,x}} \bigl(c^{-1/2} - e^{\phi/2}\bigr)^2 \geq \mu_d(K \setminus D_{\phi,x})\bigl(c^{-1/2} - e^{\phi(x)/2}\bigr)^2.$$

Since $\log(1-t) \geq -2t$ for all $t \in [0, 1/2]$, we deduce that if $\mu_d(K \setminus D_{\phi,x}) \geq 4\delta^2 c$, then

$$\phi(x) \geq 2\log\left(1 - \frac{\delta c^{1/2}}{\mu_d(K \setminus D_{\phi,x})^{1/2}}\right) - \log c \geq -\frac{4\delta c^{1/2}}{\mu_d(K \setminus D_{\phi,x})^{1/2}} - \log c,$$

as required. Turning to assertions (ii) and (iii), we suppose for now that $\mu_d(K) = 1$ and begin by establishing that:

Claim. *There exists $s_d > 0$, depending only on d, such that $\phi_0 := \log f_0 \leq \log(s_d \log^d(e\theta) - s_d + 1) =: t_d(\theta)$ on K.*

Proof of Claim. Since $\phi_0 \in \Phi$ and $K \in \mathcal{K}$, we have $\sup_{x\in K} \phi_0(x) = \sup_{x\in \operatorname{Int} K} \phi_0(x)$. Indeed, for any $z \in K$, note that if $y \in \operatorname{Int} K$, then $[y, z) \subseteq \operatorname{Int} K$ (Schneider, 2014, Lemma 1.1.9), so it follows from the concavity of ϕ_0 that $\phi_0(z) \leq \sup_{x\in[y,z)} \phi_0(x) \leq \sup_{x\in \operatorname{Int} K} \phi_0(x)$. Thus, it will suffice to show that a bound of the above form holds on $\operatorname{Int} K$.

Fix $x \in \operatorname{Int} K$ and assume that $a := \phi_0(x) + \log\theta > 0$, for otherwise there is nothing to prove. Now $K - x \in \mathcal{K}$ and $0 \in \operatorname{Int}(K - x)$, so as remarked at the start of Section 2.7, the Minkowski functional $\rho_{K-x} : w \mapsto \inf\{\lambda > 0 : w \in \lambda(K-x)\} \in [0, \infty)$ is convex. Thus, the function $\psi_0 : \mathbb{R}^d \to \mathbb{R}$ defined by

$$\psi_0(w) := a\bigl(1 - \rho_{K-x}(w - x)\bigr) - \log\theta$$

is concave, and note that the restriction of ψ_0 to any ray with endpoint x is an affine function. Also, $\psi_0(x) = \phi_0(x)$, and since $f_0 \geq \theta^{-1} f_K = \theta^{-1}$ on K by hypothesis, we have $\psi_0(w) = -\log\theta \leq \phi_0(w)$ for all $w \in \partial K$. Since ϕ_0 is concave, this implies that $-\log\theta \leq \psi_0 \leq \phi_0$ on K. Recalling that f_0 is a density and setting $g(r) := \theta^{-1}e^{a(1-r)}$ for $r \geq 0$ in Xu and Samworth (2021, Lemma S1), we deduce that

$$1 \geq \int_K e^{\phi_0} \geq \int_K e^{\psi_0} = \theta^{-1} d \int_0^1 r^{d-1} e^{a(1-r)}\, dr = \theta^{-1}\frac{d!\, e^a}{a^d}\gamma(d, a) = \theta^{-1}\sum_{\ell=0}^{\infty} \frac{d!}{(\ell + d)!} a^\ell, \quad (2.7.11)$$

where $\gamma(d, a)$ is defined as in (2.7.6) and the second equality above follows by similar reasoning to that used to obtain (2.7.9). The final expression in (2.7.11) is bounded below by $\{1 + a/(d + 1)\}/\theta$, so

$$\phi_0(x) = a - \log\theta \leq (d + 1)(\theta - 1) - \log\theta \leq (d + 1)(\theta - 1). \quad (2.7.12)$$

Suppose now that $a \geq 1$. Since $s \mapsto \sum_{\ell=0}^{\infty} d!\, s^\ell/(\ell + d)!$ is increasing on $[0, \infty)$, it follows from (2.7.11) that $\theta \geq d!\, e\gamma(d, 1) =: \theta_d$. In addition, introducing random variables $W \sim \operatorname{Po}(1)$ and $W_a \sim \operatorname{Po}(a)$, we see that $\gamma(d, a) = \mathbb{P}(W_a \geq d) \geq \mathbb{P}(W \geq d) = \gamma(d, 1)$. Thus, defining $l : (0, \infty) \to \mathbb{R}$ by $l(s) := e^s/s^d$, we deduce from (2.7.11) that

$$l(a) = \frac{e^a}{a^d} \leq \frac{\theta}{d!\, \gamma(d, 1)}. \quad (2.7.13)$$

Observe now that there exists $C_d > 1$, depending only on d, such that for all $\tilde{\theta} \geq \theta_d$, we have $\log(C_d\,\tilde{\theta}\log^d\tilde{\theta}) \geq d$ and $d!\,\gamma(d,1)C_d\log^d\tilde{\theta} \geq 2^{d-1}\bigl(\log^d C_d + \log^d(\tilde{\theta}\log^d\tilde{\theta})\bigr) \geq \log^d(C_d\,\tilde{\theta}\log^d\tilde{\theta})$, so that

$$l\bigl(\log(C_d\,\tilde{\theta}\log^d\tilde{\theta})\bigr) = \frac{C_d\,\tilde{\theta}\log^d\tilde{\theta}}{\log^d(C_d\,\tilde{\theta}\log^d\tilde{\theta})} \geq \frac{\tilde{\theta}}{d!\,\gamma(d,1)}. \tag{2.7.14}$$

Since l is increasing on $[d,\infty)$, it follows from (2.7.13) and (2.7.14) that

$$\phi_0(x) = a - \log\theta \leq \log_+(C_d\log^d\theta), \tag{2.7.15}$$

provided that $\phi_0(x) + \log\theta = a \geq 1$. In fact, (2.7.15) holds even when $a < 1$, so in all cases, we deduce from this and (2.7.12) that $\phi_0(x) \leq \min\{(d+1)(\theta-1), \log_+(C_d\log^d\theta)\}$. Note that there exists $\tilde{\theta}_d > 1$, depending only on d, such that $(d+1)(\tilde{\theta}-1) \geq \log_+(C_d\log^d\tilde{\theta})$ for all $\tilde{\theta} \geq \tilde{\theta}_d$. Also, since $\tilde{\theta} \mapsto \log^d(e\tilde{\theta}) - 1$ is increasing and has strictly positive derivative at $\tilde{\theta} = 1$, we have $e^{(d+1)(\tilde{\theta}-1)} - 1 \lesssim_d \tilde{\theta} - 1 \lesssim_d \log^d(e\tilde{\theta}) - 1$ for all $\tilde{\theta} \in [1, \tilde{\theta}_d]$. We conclude that there exists $s_d \geq 1$, depending only on d, such that $\phi_0(x) \leq \log(s_d\log^d(e\theta) - s_d + 1)$, as required. □

Proceeding with the proofs of (ii) and (iii), we may assume without loss of generality that $\operatorname{supp} f = \operatorname{dom}\phi \subseteq K$, since otherwise we can replace f by $f\mathbb{1}_K$; indeed, the hypotheses and conclusions depend on f only through $f|_K$. Then $\sqrt{f_0} - e^{\phi/2} \geq \theta^{-1/2}$ on $K\setminus\operatorname{dom}\phi$ under our assumption that $\mu_d(K) = 1$, so $\delta^2 \geq \int_K(\sqrt{f_0} - e^{\phi/2})^2 \geq \theta^{-1}\mu_d(K\setminus\operatorname{dom}\phi) = \theta^{-1}\bigl(1 - \mu_d(\operatorname{dom}\phi)\bigr)$. Since $\operatorname{dom}\phi$ is convex, this implies that $\operatorname{Int}\operatorname{dom}\phi$ is non-empty, and since ϕ is concave, it follows as in the first paragraph of the proof of the Claim above that $\sup_{x\in K}\phi(x) = \sup_{x\in\operatorname{dom}\phi}\phi(x) = \sup_{x\in\operatorname{Int}\operatorname{dom}\phi}\phi(x)$. Thus, it will suffice to show that the bounds in (ii) and (iii) hold on $\operatorname{Int}\operatorname{dom}\phi$.

Fix $x \in \operatorname{Int}\operatorname{dom}\phi$ and assume that $\phi(x) > t \equiv t_d(\theta)$, for otherwise there is nothing to prove. Since ϕ is upper semi-continuous, the set $L := \{u \in K : \phi(u) \geq t\}$ is compact and convex (Rockafellar, 1997, Theorem 7.1), and since ϕ is continuous on $\operatorname{Int}\operatorname{dom}\phi$ (Schneider, 2014, Theorem 1.5.3), we have $x \in \operatorname{Int} L$. Thus, $L - x \in \mathcal{K}$ and $0 \in \operatorname{Int}(L-x)$, so the Minkowski functional $\rho_{L-x}\colon \mathbb{R}^d \to [0,\infty)$ is convex. Since $b := \phi(x) - t > 0$, the function $\psi\colon \mathbb{R}^d \to \mathbb{R}$ defined by

$$\psi(w) := b\bigl(1 - \rho_{L-x}(w-x)\bigr) + t$$

is concave, and as was the case for the function ψ_0 defined in the proof of the Claim, the restriction of ψ to any ray with endpoint x is an affine function. Also, $\psi(x) = \phi(x)$ and $\psi(w) = t \leq \phi(w)$ for all $w \in \partial L$, so by the Claim above and the concavity of ϕ, we deduce that

$$\phi_0 \leq t \leq \psi \leq \phi \;\text{ on } L, \text{ and} \tag{2.7.16}$$

$$\phi_0 \geq -\log\theta \geq t - \beta b \geq \psi \geq \phi \;\text{ on } K \setminus \bigl(x + (1+\beta)(L-x)\bigr) \tag{2.7.17}$$

for all $\beta \geq (t + \log\theta)/b$. Now fix any $\alpha \in (0,1)$ and suppose first that $\mu_d(L) \geq \alpha$. By applying (2.7.16) and setting $g(r) := b^2(1-r)^2$ for $r \geq 0$ in Xu and Samworth (2021, Lemma S1), we find that

$$\begin{aligned}\delta^2 \geq \int_L (e^{\phi/2} - e^{\phi_0})^2 \geq \int_L (e^{\psi/2} - e^{t/2})^2 \geq e^t\int_L\frac{(\psi-t)^2}{4} &= \frac{d\mu_d(L)e^t}{4}\int_0^1 b^2(1-r)^2\,r^{d-1}\,dr \\ &\geq \frac{\alpha e^t}{2(d+1)(d+2)}\,b^2. \end{aligned}\tag{2.7.18}$$

On the other hand, suppose instead that $\mu_d(L) < \alpha$. Fix $\beta \geq (t + \log\theta)/b$, and let $t' := t - \beta b$ and $L_\beta := x + (1+\beta)(L-x)$. Then $\mu_d(K\setminus L_\beta) \geq \mu_d(K) - \mu_d(L_\beta) = 1 - (1+\beta)^d\,\mu_d(L) > 1 - (1+\beta)^d\,\alpha$.

Together with (2.7.17), this implies that

$$\delta^2 \geq \int_{K\setminus L_\beta} \bigl(e^{\phi_0/2} - e^{\phi/2}\bigr)^2 \geq \mu_d(K\setminus L_\beta)\bigl(\theta^{-1/2} - e^{t'/2}\bigr)^2 \geq \biggl\{1 - \biggl(1 + \frac{t-t'}{b}\biggr)^d \alpha\biggr\}\bigl(\theta^{-1/2} - e^{t'/2}\bigr)^2. \tag{2.7.19}$$

To obtain the bounds in (ii) and (iii), we now substitute suitably chosen values of α and β into (2.7.18) and (2.7.19). For (ii), let $\alpha = 1/4$ and $\beta = 2^{1/d} - 1$. Since $t = 0$, it follows from (2.7.18) that if $\mu_d(L) \geq 1/4$, then $\phi(x) = b \leq \sqrt{8(d+1)(d+2)}\,\delta$. Otherwise, if $\mu_d(L) < 1/4$, then since $\theta = 1$ and $t' = -\beta\phi(x)$, we deduce from (2.7.19) that

$$\begin{aligned}\phi(x) \leq -\frac{2}{\beta}\log(1-\sqrt{2}\delta) \leq \frac{2\sqrt{2}\delta}{\beta(1-\sqrt{2}\delta)} &= \frac{2\sqrt{2}\delta}{1-\sqrt{2}\delta}\Bigl(1 + 2^{1/d} + \ldots + 2^{(d-1)/d}\Bigr)\\ &\leq 4\sqrt{2}\delta\cdot 2d = (8\sqrt{2}d)\delta,\end{aligned}$$

where the second inequality above follows since $\delta \in (0, 2^{-3/2}]$ by assumption. Therefore, (ii) holds when $\mu_d(K) = 1$. As for (iii), suppose that $\theta > 1$, and let $\alpha = (\delta/d)^{2d/(d+2)}e^{-t}/4 \in (0, 1/4)$ and $\beta = \{t + \log(4\theta)\}/b$, so that $t' = -\log(4\theta)$. If $\mu_d(L) \geq \alpha$, then $\phi(x) - t = b \leq \sqrt{8(d+1)(d+2)}\,d^{\,d/(d+2)}\delta^{2/(d+2)} \lesssim (d^{\,d+1}\delta)^{2/(d+2)}$ by (2.7.18). Otherwise, if $\mu_d(L) < \alpha$, then since $8\theta\delta^2 \leq 1$ by assumption, we deduce from (2.7.19) that

$$\biggl(1 + \frac{t + \log(4\theta)}{b}\biggr)^d \alpha \geq 1 - \frac{\delta^2}{(\theta^{-1/2}/2)^2} = 1 - 4\theta\delta^2 \geq 1/2.$$

Now since $\alpha \leq 1/4$, we have $(2\alpha)^{-1/d} - 1 \geq (1 - 2^{-1/d})(2\alpha)^{-1/d} \geq \alpha^{-1/d}/(4d) > 0$, so by rearranging the inequality above, we conclude that

$$b \leq \frac{t + \log(4\theta)}{(2\alpha)^{-1/d} - 1} \leq 4d\alpha^{1/d}\bigl(t + \log(4\theta)\bigr) \leq 4d^{\,d/(d+2)}\delta^{2/(d+2)}\,\frac{t + \log(4\theta)}{e^{t/d}}. \tag{2.7.20}$$

Recalling that $e^{t_d(\tilde\theta)} = s_d\log^d(e\tilde\theta) - s_d + 1 \geq \log^d(e\tilde\theta)$ for all $\tilde\theta \in [1,\infty)$ and that $se^{-s/d} \leq d/e$ for all $s \in [0,\infty)$, we see that there exists a universal constant $C' > 0$ such that $\{t_d(\tilde\theta) + \log(4\tilde\theta)\}/e^{t_d(\tilde\theta)/d} \leq C'd$ for all $\tilde\theta \in [1,\infty)$. Together with (2.7.20), this implies that $\phi(x) - t = b \lesssim (d^{\,d+1}\delta)^{2/(d+2)}$ when $\mu_d(L) < \alpha$. This completes the proof of (iii) in the special case where $\mu_d(K) = 1$.

Having established (ii) and (iii) under the assumption that $\mu_d(K) = 1$, we now extend these results to arbitrary $K \in \mathcal{K}^b$ by means of a simple scaling argument. For a general $K \in \mathcal{K}^b$, suppose that K, θ, f_0, f satisfy the conditions of the lemma and that $\delta \in (0, (8\theta)^{-1/2}]$. Let $\lambda := \mu_d(K)^{1/d}$ and $K' := \lambda^{-1}K$, so that $\mu_d(K') = 1$. Then defining $\tilde f_0, \tilde f\colon \mathbb{R}^d \to [0,\infty)$ by $\tilde f_0(x) := \lambda^d f_0(\lambda x)$ and $\tilde f(x) := \lambda^d f(\lambda x)$, we see that $\tilde f_0 \in \mathcal{F}$ and $\tilde f \in \mathcal{G}$. Moreover, $\tilde f_0(x) \geq \lambda^d\theta^{-1}f_K(\lambda x) = \theta^{-1}f_{K'}(x)$ for all $x \in K'$ and $\int_{K'}\bigl(\tilde f^{1/2} - \tilde f_0^{1/2}\bigr)^2 = \int_K\bigl(f^{1/2} - f_0^{1/2}\bigr)^2 \leq \delta^2$. This shows that $K', \theta, \tilde f_0, \tilde f$ satisfy the conditions of the lemma. Now for any $x \in K$, we have $\lambda^{-1}x \in K'$, and since $\mu_d(K') = 1$, it follows from the bounds obtained hitherto that

$$\log f(x) + \log\mu_d(K) = \log f(x) + \log(\lambda^d) = \log\tilde f(\lambda^{-1}x) \leq \begin{cases}(8\sqrt{2}d)\delta & \text{if } \theta = 1\\ t_d(\theta) + s'(d^{\,(d+1)}\delta)^{2/(d+2)} & \text{if } \theta > 1,\end{cases}$$

as required. □

In addition, we derive a lower bound on $\sup_{x\in K^+_{\alpha,1}}\{\phi(x) + \alpha^\top x + \log c_{K,\alpha}\}$ that holds whenever $\phi \in \Phi$ and e^ϕ is close in Hellinger distance to some $f_{K,\alpha} \in \mathcal{F}^1_\star$ with $\alpha \neq 0$. For $d \in \mathbb{N}$, define

$\nu_d := \{2^{-3}d^{-d}e^{-1}\gamma(d,1)\}^{1/2}$, where $\gamma(d,1)$ is taken from Lemma 2.7.6. Recall the definitions of $K_{\alpha,t}^+$ and $c_{K,\alpha}$ from (2.7.1) and Proposition 2.7.4 respectively.

Lemma 2.7.15. *Fix $f_{K,\alpha} \in \mathcal{F}_\star^1$ with $K \in \mathcal{K}$ and $\alpha \neq 0$. For $\phi \in \Phi$, define $\tilde{\phi}_{K,\alpha} \colon \mathbb{R}^d \to [-\infty,\infty)$ by $\tilde{\phi}_{K,\alpha} := \phi(x) + \alpha^\top x + \log c_{K,\alpha}$. If $\int_K \bigl(e^{\phi/2} - f_{K,\alpha}^{1/2}\bigr)^2 \leq \delta^2$ for some $\delta \in (0,\nu_d]$, then there exists $x_- \in K_{\alpha,1}^+$ such that $\tilde{\phi}_{K,\alpha}(x_-) > -2$.*

Proof. Let $\psi := \tilde{\phi}_{K,\alpha}$. We first establish that there exists $x_- \in K' := K_{\alpha,1}^+$ with the property that $\mu_d(K' \cap H^+) \geq 2^{-1}d^{-d}\mu_d(K')$ whenever H^+ is a half-space whose boundary contains x_-. Then we show that any such x_- necessarily satisfies $\psi(x_-) \geq -2$. To justify the first claim above, we apply Fritz John's theorem (John, 1948), which asserts that there exists an invertible affine map $T \colon \mathbb{R}^d \to \mathbb{R}^d$ such that $\bar{B}(0,1/d) \subseteq \tilde{K} := T(K') \subseteq \bar{B}(0,1)$. Now if H^+ is any hyperplane whose boundary contains 0, then $\mu_d(\tilde{K} \cap H^+) \geq 2^{-1}\mu_d(\bar{B}(0,1/d)) = 2^{-1}d^{-d}\mu_d(\bar{B}(0,1)) \geq 2^{-1}d^{-d}\mu_d(\tilde{K})$, so $x_- := T^{-1}(0) \in K'$ has the required property.

We may now assume that $\psi(x) \leq 0$ for every $x \in K'$, since otherwise the desired conclusion follows trivially. Then $\psi \in \Phi$ and $e^{\psi(u)/2} \leq e^{\psi(x_-)/2} \leq 1$ for all $u \in K' \setminus D_{\psi,x_-} \subseteq K$, so

$$
\begin{aligned}
\delta^2 &\geq \int_{K'\setminus D_{\psi,x_-}} \bigl(f_{K,\alpha}^{1/2} - e^{\phi/2}\bigr)^2 \\
&= \int_{K'\setminus D_{\psi,x_-}} \frac{e^{-\alpha^\top u}}{c_{K,\alpha}} \bigl(1 - e^{\psi(u)/2}\bigr)^2 \, du \geq (1 - e^{\psi(x_-)/2})^2 \int_{K'\setminus D_{\psi,x_-}} \frac{e^{-\alpha^\top u}}{c_{K,\alpha}} \, du.
\end{aligned}
$$

Since $x_- \notin D_{\psi,x_-}$ and D_{ψ,x_-} is convex, the separating hyperplane theorem (Schneider, 2014, Theorem 1.3.4) implies that there exists a open half-space H^+ such that $x_- \in \partial H^+$ and $K' \cap H^+ \subseteq K' \setminus D_{\psi,x_-}$. In view of the defining property of x_- and Lemma 2.7.6, it follows that

$$
\int_{K'\setminus D_{\psi,x_-}} \frac{e^{-\alpha^\top u}}{c_{K,\alpha}} \, du \geq \int_{K'\cap H^+} \frac{e^{-\alpha^\top u}}{c_{K,\alpha}} \, du \geq \frac{e^{-1}\,\mu_d(K' \cap H^+)}{c_{K,\alpha}} \geq \frac{(2e)^{-1}d^{-d}\mu_d(K')}{c_{K,\alpha}} \geq 4\nu_d^2.
$$

By combining the bounds in the two previous displays, we conclude that

$$
\psi(x_-) \geq 2\log\left(1 - \frac{\delta}{2\nu_d}\right) > -2,
$$

where we have used the fact that $\delta \in (0,\nu_d]$ to obtain the final inequality. This completes the proof of the lemma. □

The remaining results in this subsection prepare the ground for the proof of Proposition 2.6.8, which establishes a local bracketing entropy bound for classes of log-concave functions f that lie within small Hellinger neighbourhoods $\mathcal{G}(f_S,\delta)$ of the uniform density f_S on a d-simplex S. As mentioned after the statement of Theorem 2.2.3 in Section 2.2, we now develop further the pointwise lower bound from Lemma 2.7.14(i) by identifying subsets (or 'invelopes') J_η^S of a d-simplex S with the property that $\mu_d(S \setminus D_{\phi,x}) \gtrsim \eta\mu_d(S)$ for all $x \in J_\eta^S$, which ensures that $\log f + \log \mu_d(S) \gtrsim -\delta/\eta^{1/2}$ for all $f \in \mathcal{G}(f_S,\delta)$. This is the purpose of Lemma 2.7.19(iii), which handles the case where S is a regular d-simplex. However, in the proof of Proposition 2.6.8, it turns out that for technical reasons, we cannot work directly with the invelopes we obtain in this lemma; instead, the strategy we pursue involves constructing polytopal approximations that satisfy the conditions of Corollary 2.7.22. For technical convenience, we first derive analogous results in the case where the domain is $[0,1]^d$ (Lemmas 2.7.17 and 2.7.21), before adapting the relevant geometric constructions to the simplicial setting described above. The volume bound in Lemma 2.7.17(iii) and the properties in Corollary 2.7.22 are exploited in the derivation of the local bracketing entropy bounds in Proposition 2.6.8, where they help to ensure that the exponent of δ matches that of ε; see the paragraph containing (2.6.42). This in turn is ultimately responsible for the essentially parametric adaptive rates that we are able to establish in Section 2.2.

Before proceeding, we make some further definitions. Fix $1 \leq k \leq d$ and let $P \subseteq \mathbb{R}^d$ be a k-simplex or a k-parallelotope. Then for each vertex v of P, there are exactly k other vertices $v_1, \ldots, v_k$ of P for which $[v, v_1], \ldots, [v, v_k]$ are edges of P. Setting $w_j := v_j - v$ for $1 \leq j \leq k$, we note that

$$P = \begin{cases} \bigl\{v + \sum_{j=1}^k \lambda_j w_j : \lambda_j \geq 0,\, \sum_{j=1}^k \lambda_j \leq 1 \text{ for all } j\bigr\} & \text{if } P \text{ is a } k\text{-simplex} \\ \bigl\{v + \sum_{j=1}^k \lambda_j w_j : 0 \leq \lambda_j \leq 1 \text{ for all } j\bigr\} & \text{if } P \text{ is a } k\text{-parallelotope.} \end{cases}$$

For any fixed $x \in \operatorname{relint} P$, there exist unique $\tilde{x}_1, \ldots, \tilde{x}_k \in (0,1)$ such that $x = v + \sum_{j=1}^k \tilde{x}_j w_j$. Then

$$P^v(x) := \bigl\{v + \textstyle\sum_{j=1}^k \lambda_j \tilde{x}_j w_j : 0 \leq \lambda_j \leq 1 \text{ for all } j\bigr\}$$

is a closed k-parallelotope, two of whose vertices are v and x. Observe that $P^v(x) \subseteq P$; indeed, if $\lambda_1, \ldots, \lambda_k \in [0,1]$, then $\lambda_j \tilde{x}_j \in [0,1]$ for all $1 \leq j \leq k$ and $\sum_{j=1}^k \lambda_j \tilde{x}_j \leq \sum_{j=1}^k \tilde{x}_j$. Also, a simple calculation shows that

$$\mu_k(P^v(x)) = \begin{cases} k!\, \mu_k(P) \prod_{j=1}^k \tilde{x}_j & \text{if } P \text{ is a } k\text{-simplex} \\ \mu_k(P) \prod_{j=1}^k \tilde{x}_j & \text{if } P \text{ is a } k\text{-parallelotope.} \end{cases} \tag{2.7.21}$$

The following elementary geometric result will be used in the proofs of Lemmas 2.7.17 and 2.7.19.

Lemma 2.7.16. *Let $P \subseteq \mathbb{R}^d$ be as above and fix $x \in \operatorname{relint} P$. If $H^+ \subseteq \mathbb{R}^d$ is a closed half-space such that $x \in \partial H^+$, then there exists a vertex v of P for which $P^v(x) \subseteq P \cap H^+$.*

Proof. Since $x \in \partial H^+$, there exists a unit vector $\theta \in \mathbb{R}^d$ such that $H^+ = \{u \in \mathbb{R}^d : \theta^\top u \leq \theta^\top x\}$, and since P is compact and convex, we can find a vertex v of P such that $v \in \operatorname{argmin}_{u \in P} \theta^\top u$. To see that v has the required property, define $v_j, w_j, \tilde{x}_j$ as above for $1 \leq j \leq k$, and observe that $\theta^\top w_j = \theta^\top(v_j - v) \geq 0$ for all j by our choice of v. Therefore, since $\tilde{x}_j > 0$ for all j, it follows from the definition of $P^v(x)$ that $\theta^\top u \leq \theta^\top x$ for all $u \in P^v(x)$, so $P^v(x) \subseteq H^+$, as required. $\square$

We now consider $Q = Q_d := [0,1]^d$. For each $\xi = (\xi_1, \ldots, \xi_d) \in \{0,1\}^d$, let $g_\xi \colon Q \to Q$ be the function $(x_1, \ldots, x_d) \mapsto (\xi_1 + (-1)^{\xi_1} x_1, \ldots, \xi_d + (-1)^{\xi_d} x_d)$. Then $G_R(Q) \equiv G_R(Q_d) := \{g_\xi : \xi \in \{0,1\}^d\}$ is the subgroup of (affine) isometries of Q generated by reflections in the affine hyperplanes $\{(w_1, \ldots, w_d) \in \mathbb{R}^d : w_j = 1/2\}$, where $j = 1, \ldots, d$. We say that $D \subseteq [0,1]^d$ is $G_R(Q)$*-invariant* if $g(D) = D$ for all $g \in G_R(Q)$.

Moreover, let $M \colon Q \to [0,1/2]^d$ be the function $(x_1, \ldots, x_d) \mapsto (x_1 \wedge (1 - x_1), \ldots, x_d \wedge (1 - x_d))$. Then for each $x \in Q$, note that $M(x)$ is an element of the orbit of x under $G_R(Q)$ that lies in $[0,1/2]^d$, and also that $M(g(x)) = M(x)$ for all $g \in G_R(Q)$.

Lemma 2.7.17. *For each $\eta > 0$, the sets $A_\eta \equiv A_{d,\eta} := \{(x_1, \ldots, x_d) \in (0,\infty)^d : \prod_{j=1}^d x_j \geq \eta\}$ and $J_\eta \equiv J_{d,\eta} := \{x \in Q : M(x) \in A_\eta\}$ are closed and convex, and have the following properties:*

(i) $A_\eta = A_{d,\eta} = \eta^{1/d} A_{d,1}$ *and* $[0,1/2]^d \cap J_\eta = [0,1/2]^d \cap A_\eta$.

(ii) $J_\eta = \bigcap_{g \in G_R(Q)} g(A_\eta \cap Q)$*, so* J_η *is* $G_R(Q)$*-invariant.*

(iii) If $\eta \leq 2^{-d}$*, then* $\mu_d(Q \setminus J_\eta) = 2^d \eta \sum_{\ell=0}^{d-1} \log^\ell(2^{-d}\eta^{-1})/\ell!$ *and therefore* $\mu_d(Q \setminus J_{\alpha\eta}) \leq \alpha \mu_d(Q \setminus J_\eta)$ *for all* $\alpha \geq 1$.

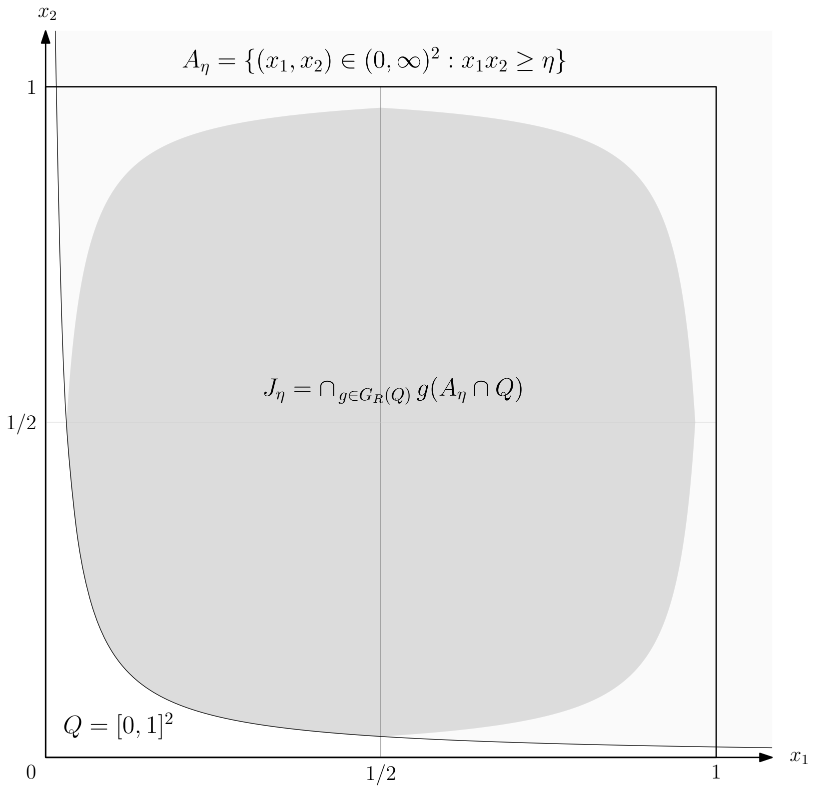

Figure 2.4: Illustration of the sets A_η (union of the lighter and darker regions) and J_η (darker region) in Lemma 2.7.17 when $d = 2$.

(iv) If $C \subseteq Q$ is convex and $J_\eta \not\subseteq \operatorname{Int} C$, then $\mu_d(Q \setminus C) \geq \eta$.

(v) If $\phi \in \Phi$ and $\delta, \eta > 0$ are such that $4\delta^2 \leq \eta \leq 2^{-d}$ and $\int_Q (e^{\phi/2} - 1)^2 \leq \delta^2$, then $\phi(x) \geq -4\delta\eta^{-1/2}$ for all $x \in J_\eta$.

Proof. The assertions in (i) are immediate from the definitions above. In addition, the function $r\colon (0,\infty)^d \to (0,\infty)$ defined by $r(x_1,\ldots,x_d) := \prod_{j=1}^d x_j^{-1}$ is convex since its Hessian matrix is positive definite everywhere, so $A_\eta = \{x \in (0,\infty)^d : r(x) \leq \eta^{-1}\}$ is convex for all $\eta > 0$. Now for $x \in Q$, note that if $M(x) \in A_\eta$ (i.e. $x \in J_\eta$), then $g(x) \in A_\eta$ for all $g \in G_R(Q)$ by the definition of M, and since $M(x) = \tilde{g}(x)$ for some $\tilde{g} \in G_R(Q)$, the converse is also true. This shows that $J_\eta = \bigcap_{g\in G_R(Q)} g(A_\eta \cap Q)$, as claimed in (ii), and since $g(A_\eta \cap Q)$ is convex for all $g \in G_R(Q)$, we see that J_η is convex for all $\eta > 0$.

Turning to (iii), the formula for $\mu_d(Q\setminus J_\eta)$ certainly holds when $d = 1$, and we now extend this to all $d \geq 1$ by induction. For $d \geq 2$, we partition $[0,1/2]^d$ into the sets $D_1 := [0,1/2]^{d-1} \times [0, 2^{d-1}\eta) \subseteq J_\eta^c$ and $D_2 := [0,1/2]^{d-1} \times [2^{d-1}\eta, 1/2]$, and write

$$\begin{aligned}\mu_d([0,1/2]^d \setminus J_\eta) = \mu_d(D_1) + \mu_d(D_2 \setminus J_\eta) &= \eta + \int_{2^{d-1}\eta}^{1/2} \frac{\eta}{x_d} \sum_{\ell=0}^{d-2} \log^\ell\biggl(\frac{x_d}{2^{d-1}\eta}\biggr)\frac{1}{\ell!}\,dx_d \\ &= \eta + \eta\sum_{\ell=1}^{d-1} \log^\ell(2^{-d}\eta^{-1})\frac{1}{\ell!},\end{aligned}$$

where we have used the inductive hypothesis to obtain the integrand above. Since $\mu_d(J_\eta) = 2^d\mu_d([0,1/2]^d \setminus J_\eta)$ by symmetry, this completes the inductive step. In particular, $\mu_d(Q \setminus J_\eta) \geq 2^d\eta$ when $\eta \leq 2^{-d}$. It follows from this and the formula for $\mu_d(Q \setminus J_\eta)$ that $\mu_d(Q \setminus J_{\alpha\eta}) \leq \alpha\mu_d(Q \setminus J_\eta)$

for all $\alpha \geq 1$, including when $\alpha\eta \geq 2^{-d}$, in which case $\mu_d(Q \setminus J_{\alpha\eta}) = 1$. Alternatively, to obtain the final assertion of (iii), simply note that $[0,1/2]^d \setminus J_{\alpha\eta} \subseteq \alpha^{1/d}\,([0,1/2]^d \setminus J_\eta)$ for all $\alpha \geq 1$ and $\eta > 0$.

To establish (iv), fix a convex set $C \subseteq Q$ and suppose that there exists $x \in J_\eta \setminus \operatorname{Int} C$. By the separating hyperplane theorem, there is a closed half-space H^+ such that $x \in \partial H^+$ and $C \cap \operatorname{Int} H^+ = \emptyset$. Since $x \in \operatorname{Int} Q$, it follows from Lemma 2.7.16 that there exists a vertex v of Q such that $Q^v(x) \subseteq Q \cap H^+$. Therefore, $\mu_d(Q \setminus C) \geq \mu_d(Q \cap H^+) \geq \mu_d(Q^v(x)) = \prod_{j=1}^d |x_j - v_j| \geq \eta$ by (2.7.21), as desired.

Finally, for fixed $x \in J_\eta$ and $\eta \geq 4\delta^2$, let $C := Q \cap D_{\phi,x}$. Since $x \in J_\eta \setminus \operatorname{Int} C$ by the definition of $D_{\phi,x}$, it follows from (iv) that $\mu_d(Q \setminus D_{\phi,x}) \geq \eta$, and we deduce from Lemma 2.7.14(i) that $\phi(x) \geq -4\delta\, \mu_d(Q \setminus D_{\phi,x})^{-1/2} \geq -4\delta\eta^{-1/2}$, as required. $\square$

We now obtain an analogous result for $\triangle \equiv \triangle_d := \operatorname{conv}\{e_1, \dots, e_{d+1}\} \subseteq \mathbb{R}^{d+1}$, a regular d-simplex of side length $\sqrt{2}$ that will be viewed as a subset of its affine hull $\operatorname{aff} \triangle = \{x = (x_1, \dots, x_{d+1}) \in \mathbb{R}^{d+1} : \sum_{j=1}^{d+1} x_j = 1\}$. Note that $\triangle$ can be subdivided into $d+1$ congruent polytopes $R_1, \dots, R_{d+1}$, where

$$R_j := \bigl\{(x_1, \dots, x_{d+1}) \in \triangle : x_j = \max_{1 \leq \ell \leq d+1} x_\ell\bigr\}. \tag{2.7.22}$$

The proof of Lemma 2.7.19 makes use of another elementary fact from linear algebra.

Lemma 2.7.18. *Fix $d \geq 2$, let $u_1, u_2 \in \mathbb{R}^d$ be unit vectors, and for $i = 1, 2$, let $H_i := \{x \in \mathbb{R}^d : u_i^\top x = 0\}$. For $x \in \mathbb{R}^d$, write $\Pi(x) := x - (u_2^\top x)u_2$ for the orthogonal projection of x onto H_2. Then $\mu_{d-1}\bigl(\Pi(A)\bigr) = |u_1^\top u_2|\, \mu_{d-1}(A)$ for all Lebesgue-measurable $A \subseteq H_1$, where $\Pi(A)$ denotes the image of A under Π.*

Proof. Let $\alpha := u_1^\top u_2$. The result holds trivially if $u_1 = u_2$, so we now assume that $u_1 \neq u_2$, in which case $H_1 \cap H_2$ has dimension $d-2$. Let B be a fixed orthonormal basis $\{v_3, \dots, v_d\}$ of $H_1 \cap H_2$ when $d \geq 3$, and otherwise set $B := \emptyset$ when $d = 2$. Define $v_1 := u_2 - \alpha u_1$ and $v_2 := -u_1 + \alpha u_2$, so that $\|v_i\|^2 = v_i^\top v_i = 1 - \alpha^2$ for $i = 1, 2$, and let $v_i' := v_i / \|v_i\|$ for each i. Then $B_i := \{v_i'\} \cup B$ is an orthonormal basis of H_i for each i, and $\Pi(v_1) = (u_2 - \alpha u_1) - (1 - \alpha^2)u_2 = \alpha v_2$, whence $\Pi(v_1') = \alpha v_2'$. Thus, Π is represented by the matrix $\operatorname{diag}(\alpha, 1, \dots, 1)$ with respect to the bases B_1 and B_2.

Now for $i = 1, 2$, let $T_i \colon \mathbb{R}^{d-1} \to H_i$ be the linear map defined by setting $T_i\, e_1 = v_i'$, and $T_i\, e_j = v_{j+1}$ for $2 \leq j \leq d-1$ when $d \geq 3$. Then $\mu_{d-1}(A) = \mu_{d-1}\bigl(T_i(A)\bigr)$ for all i and for all measurable $A \subseteq \mathbb{R}^{d-1}$. Defining $D \colon \mathbb{R}^{d-1} \to \mathbb{R}^{d-1}$ by $D(x_1, \dots, x_{d-1}) := (\alpha x_1, \dots, x_{d-1})$, we see that if R is a hyperrectangle of the form $\prod_{j=1}^{d-1} [a_j, b_j]$, then $(\Pi \circ T_1)(R) = (T_2 \circ D)(R)$ by the final observation in the previous paragraph. Thus, if $A = T_1(R)$ for some hyperrectangle $R = \prod_{j=1}^{d-1} [a_j, b_j] \subseteq \mathbb{R}^{d-1}$, then

$$\mu_{d-1}\bigl(\Pi(A)\bigr) = \mu_{d-1}\bigl((T_2 \circ D)(R)\bigr) = \mu_{d-1}\bigl(D(R)\bigr) = |\alpha|\, \mu_{d-1}(R) = |\alpha|\, \mu_{d-1}\bigl(T_1(R)\bigr) = |\alpha|\, \mu_{d-1}(A).$$

Since the Borel σ-algebra of H_1 is generated by the π-system of sets of the form $T_1(R)$, where R is a hyperrectangle, it follows that the claimed identity $\mu_{d-1}\bigl(\Pi(A)\bigr) = |\alpha|\, \mu_{d-1}(A)$ holds for all Lebesgue-measurable $A \subseteq H_1$, as required. $\square$

Remark. The key fact that underlies this result is that $|u_1^\top u_2|$ is the determinant of any matrix which represents $\Pi|_{H_1}$ with respect to orthonormal bases of H_1 and H_2. This follows from the first paragraph of the proof, which amounts to a derivation of the principal angles between H_1 and H_2 from first principles.

Lemma 2.7.19. *Let $\Pi \colon \mathbb{R}^{d+1} \to \mathbb{R}^d$ denote the projection onto the first d coordinates, so that $\Pi(x_1, \dots, x_{d+1}) := (x_1, \dots, x_d)$, and let $Q^\triangle \equiv Q_d^\triangle$ denote the image of R_{d+1} under Π. Then $Q^\triangle$ is*

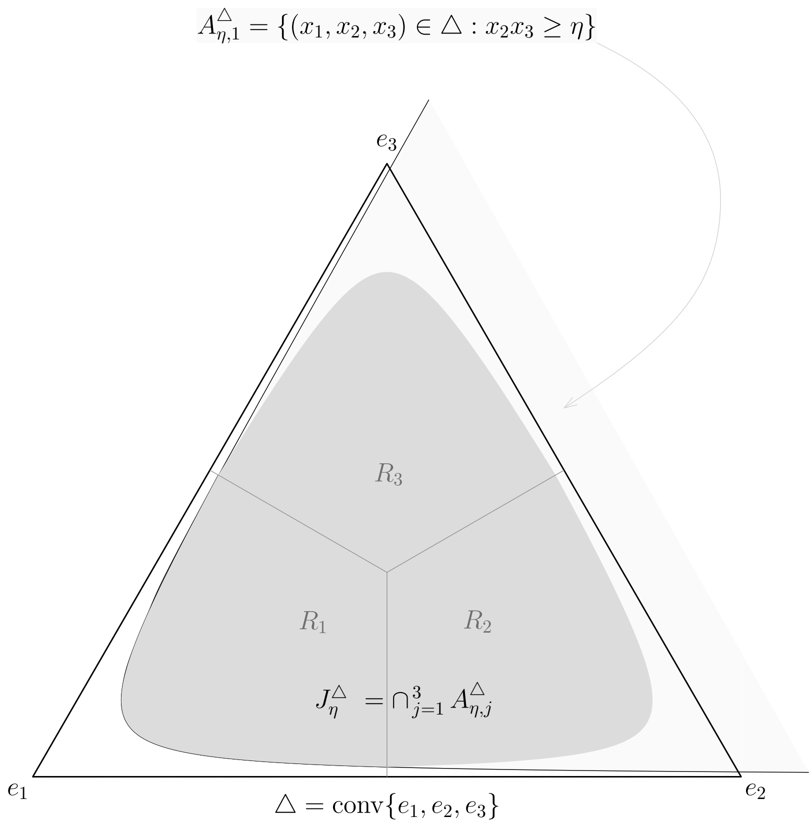

Figure 2.5: Illustration of the polytopes R_1, R_2, R_3, and the sets $A^{\triangle}_{\eta,1}$ (union of the lighter and darker regions) and $J^{\triangle}_{\eta}$ (darker region) in Lemma 2.7.19 when $d = 2$. Lemma 2.7.19(iii) is a key property that we exploit in the proof of Proposition 2.6.8; see Figure 2.1.

a polytope with $2d$ *facets, and* $[0, 1/(d+1)]^d \subseteq Q^{\triangle} \subseteq [0, 1/2]^d$. *Moreover,* $\mu_d\bigl(\Pi(A)\bigr) = \mu_d(A)/\sqrt{d+1}$ *for all Lebesgue-measurable* $A \subseteq R_{d+1}$.

In addition, for each $\eta > 0$, *the sets* $A^{\triangle}_{\eta,j} \equiv A^{\triangle}_{d,\eta,j} := \{(x_1, \ldots, x_{d+1}) \in \triangle : \prod_{\ell \neq j} x_\ell \geq \eta\}$ *and* $J^{\triangle}_{\eta} \equiv J^{\triangle}_{d,\eta} := \bigcap_{j=1}^{d+1} A^{\triangle}_{d,\eta,j}$ *are convex and have the following properties:*

(i) $\Pi(R_{d+1} \cap J^{\triangle}_{\eta}) = Q^{\triangle} \cap J_\eta$ *and* $R_j \cap J^{\triangle}_{\eta} = R_j \cap A^{\triangle}_{\eta,j}$ *for every* $1 \leq j \leq d+1$.

(ii) If $C \subseteq \triangle$ *is convex and* $J^{\triangle}_{\eta} \nsubseteq \mathrm{relint}\, C$, *then* $\mu_d(\triangle \setminus C) \geq d!\, \eta \mu_d(\triangle)$.

(iii) Suppose that $\phi, \phi_0 \colon \mathrm{aff}\, \triangle \to [-\infty, \infty)$ *are concave and upper semi-continuous, and that there exists* $\theta \in [1, \infty)$ *such that* $e^{\phi_0} \geq \bigl(\theta \mu_d(\triangle)\bigr)^{-1}$ *on* $\triangle$. *Let* $\delta, \eta > 0$ *be such that* $4\delta^2/d! \leq \eta \leq (d+1)^{-d}$ *and* $\int_{\triangle} (e^{\phi/2} - e^{\phi_0/2})^2 \leq \delta^2$. *Then*
$\phi(x) + \log \mu_d(\triangle) \geq -4\delta\{\theta/(d!\,\eta)\}^{1/2} - \log \theta$ *for all* $x \in J^{\triangle}_{\eta}$.

Proof. Note that $H := \mathrm{aff}\, \triangle = \{x = (x_1, \ldots, x_{d+1}) \in \mathbb{R}^{d+1} : \sum_{j=1}^{d+1} x_j = 1\}$ is an affine hyperplane with unit normal $u := (1/\sqrt{d+1}, \ldots, 1/\sqrt{d+1}) \in \mathbb{R}^{d+1}$. For $1 \leq k \leq d$, let $H^+_k := \{x \in \mathbb{R}^{d+1} : x_k \geq 0\}$ and $H^+_{d+k} := \{x \in \mathbb{R}^{d+1} : x_k \leq x_{d+1}\}$. Then $R_{d+1} = H \cap \bigcap_{k=1}^{2d} H^+_k \subseteq \triangle$, and it is easy to verify that $R_{d+1} \subsetneqq H \cap \bigcap_{k \neq k'} H^+_k$ for all $1 \leq k' \leq 2d$. Therefore, R_{d+1} is a polytope when viewed as a subset of H, and we deduce from Bruns and Gubeladze (2009, Theorem 1.6) that F is a facet of R_{d+1} if and only if $F = R_{d+1} \cap H^+_k$ for some $1 \leq k \leq 2d$. It follows that R_{d+1} is a polytope with exactly $2d$ facets, and since $\Pi|_H : H \to \mathbb{R}^d$ is linear and bijective, the same is true of $Q^{\triangle} = \Pi(R_{d+1})$.

To see that $[0, 1/(d+1)]^d \subseteq Q^{\triangle}$, fix $x = (x_1, \ldots, x_d) \in [0, 1/(d+1)]^d$ and define $x' := (x_1, \ldots, x_d, x_{d+1})$, where $x_{d+1} := 1 - \sum_{j=1}^{d} x_j$. Then $x_{d+1} \geq 1/(d+1) \geq x_j$ for all $1 \leq j \leq d$, so $x' \in R_{d+1} \subseteq \triangle$ and therefore $x = \Pi(x') \in \Pi(R_{d+1}) = Q^{\triangle}$, as required. In addition, if $x' = (x_1, \ldots, x_{d+1}) \in R_{d+1}$, then $0 \leq x_k \leq x_{d+1}$ and $x_k + x_{d+1} \leq \sum_{j=1}^{d+1} x_j = 1$ for all $1 \leq k \leq d$, so $x_k \in [0, 1/2]$ for all such k. It follows that $\Pi(x') \in [0, 1/2]^d$ for all $x' \in R_{d+1}$ and hence that $Q^\triangle \subseteq [0, 1/2]^d$.

Furthermore, to establish that $\mu_d\big(\Pi(A)\big) = \mu_d(A)/\sqrt{d+1}$ for all Lebesgue-measurable $A \subseteq R_{d+1}$, we apply Lemma 2.7.18 to the hyperplanes $H - e_1 = \{x \in \mathbb{R}^{d+1} : u^\top x = 0\}$ and $\{x \in \mathbb{R}^{d+1} : e_{d+1}^\top x = 0\}$, whose unit normals u and e_{d+1} satisfy $|e_{d+1}^\top u| = 1/\sqrt{d+1}$. Since Π is linear and Lebesgue measure is translation invariant, we see that

$$\mu_d\big(\Pi(A)\big) = \mu_d(\Pi(A) - e_1) = \mu_d\big(\Pi(A - e_1)\big) = \mu_d(A - e_1)/\sqrt{d+1} = \mu_d(A)/\sqrt{d+1}$$

for all Lebesgue-measurable $A \subseteq R_{d+1}$, as required.

As for (i), note that if $x' = (x_1, \dots, x_{d+1}) \in R_j \cap A_{\eta,j}^\triangle$ for some $1 \le j \le d+1$, then $x_j = \max_{1 \le \ell \le d+1} x_\ell$ and $\prod_{\ell \ne j} x_\ell \ge \eta$, so $\prod_{\ell \ne j'} x_\ell \ge \prod_{\ell \ne j} x_\ell \ge \eta$ for all $1 \le j' \le d+1$, and therefore $x' \in R_j \cap A_{\eta,j'}^\triangle$ for all j'. This shows that $R_j \cap A_{\eta,j}^\triangle \subseteq R_j \cap J_\eta^\triangle$ for each $1 \le j \le d+1$, and the reverse inclusion is clear. To see that $\Pi(R_{d+1} \cap J_\eta^\triangle) = Q^\triangle \cap J_\eta$, first note that since $Q^\triangle \subseteq [0, 1/2]^d$, it follows from Lemma 2.7.17(i) that $Q^\triangle \cap A_\eta = Q^\triangle \cap J_\eta$. Thus, $x \in Q^\triangle \cap J_\eta = Q^\triangle \cap A_\eta$ if and only if $x = \Pi(x')$ for some $x' = (x_1, \dots, x_{d+1}) \in R_{d+1}$ with $\prod_{j=1}^d x_j \ge \eta$, i.e. precisely when $x \in \Pi(R_{d+1} \cap A_{\eta,d+1}^\triangle) = \Pi(R_{d+1} \cap J_\eta^\triangle)$, as required.

The proof of (ii) is very similar to that of Lemma 2.7.17(iv). Suppose that $C \subseteq \triangle$ is convex and that there exists $x \in J_\eta^\triangle \setminus \operatorname{relint} C$. Then it once again follows from the separating hyperplane theorem and Lemma 2.7.16 that there exists a vertex v of $\triangle$ such that $\triangle^v(x) \subseteq \triangle \cap H^+$ for some closed half-space $H^+ \subseteq \mathbb{R}^{d+1}$ with $x \in \partial H^+$, $H \ne \partial H^+$ and $C \cap \operatorname{Int} H^+ = \emptyset$. Then $v = e_k$ for some $1 \le k \le d+1$, and note that $x = \sum_{j=1}^{d+1} x_j e_j = e_k + \sum_{j \ne k} x_j (e_j - e_k)$. Thus,

$$\mu_d(\triangle \setminus C) \ge \mu_d(\triangle \cap H^+) \ge \mu_d\big(\triangle^v(x)\big) = d!\,\mu_d(\triangle) \textstyle\prod_{j \ne k} x_j \ge d!\,\eta\mu_d(\triangle)$$

by (2.7.21) and the fact that $x \in J_\eta^\triangle$, as required. The final assertion (iii) follows from (ii) and Lemma 2.7.14(i) in much the same way that Lemma 2.7.17(v) follows from Lemma 2.7.17(iv). $\square$

In view of Lemma 2.7.17(iv) and Lemma 2.7.19(ii), we shall henceforth refer to the sets J_η and $J_\eta^\triangle$ as *(convex) invelopes*. Next, we show that the sets $J_\eta \subseteq Q$ can be approximated from within by polytopes P_η satisfying $\mu_d(Q \setminus P_\eta) \lesssim_d \mu_d(Q \setminus J_\eta)$, in such a way that the number of vertices of P_η does not grow too quickly as $\eta \searrow 0$. This is the content of Lemma 2.7.21, whose proof hinges on an inductive construction based on the following fact.

Lemma 2.7.20. *Let $E \subseteq (0, \infty)^d$ be a convex set with the property that $\lambda E \subseteq E$ for all $\lambda \ge 1$, and let $h\colon [0, \infty) \to [0, \infty]$ be a convex function. Then*

$$\begin{aligned} E^h := \{(x, z) \in (0, \infty)^d \times (0, \infty) : h(z) \in (0, \infty),\, x/h(z) \in E\} \\ \cup \{(x, z) \in (0, \infty)^d \times (0, \infty) : h(z) = 0,\, x \in \textstyle\bigcup_{\lambda > 0} \lambda E\} \end{aligned}$$

is a convex subset of $\mathbb{R}^{d+1} \cong \mathbb{R}^d \times \mathbb{R}$. Suppose further that E is closed and $(0, \infty)^d = \bigcup_{\lambda > 0} \lambda E$. Then $\tau_E(x) := \sup\{\lambda > 0 : x \in \lambda E\}$ lies in $(0, \infty)$ for all $x \in (0, \infty)^d$ and $\tau_E(\lambda x) = \lambda \tau_E(x)$ for all $x \in (0, \infty)^d$ and $\lambda \in (0, \infty)$. Moreover, we have the following:

(i) $\lambda E = \{x \in (0, \infty)^d : \tau_E(x) \ge \lambda\}$ and $\lambda \operatorname{Int} E = \{x \in (0, \infty)^d : \tau_E(x) > \lambda\}$ for all $\lambda > 0$, so τ_E is continuous on $(0, \infty)^d$ and $\lambda E \subsetneqq E$ for all $\lambda > 1$.

(ii) $E^h = \{(x, z) \in (0, \infty)^d \times (0, \infty) : \tau_E(x) \ge h(z)\}$.

If in addition h is lower semi-continuous and decreasing on $[0, \infty)$, and if $\lim_{x \searrow 0} h(x) = \infty$, then *(iii)* $h^{-1}(c) := \inf\{z \in [0,\infty) : h(z) \leq c\} \in (0,\infty]$ *for all* $c \in [0,\infty)$*, where we set* $\inf\emptyset := \infty$*. The function* $h^{-1}\colon [0,\infty) \to (0,\infty]$ *is convex, decreasing and lower semi-continuous. For* $z, c \in [0,\infty)$*, we have* $h(z) \leq c$ *if and only if* $h^{-1}(c) \leq z$*.*

(iv) $h^{-1} \circ \tau_E\colon (0,\infty)^d \to [0,\infty]$ *is a convex function whose epigraph is* E^h*. If* $h(z) \in (0,\infty)$ *for all* $z \in (0,\infty)$*, then* E^h *is closed and* $h^{-1} \circ \tau_E$ *is lower semi-continuous.*

(v) $\lambda E^h \subseteq E^h$ *for all* $\lambda \geq 1$*, and if* h *is not identically* ∞*, then* $(0,\infty)^{d+1} = \bigcup_{\lambda>0} \lambda E^h$*.*

Proof. Fix $(x_1,z_1),(x_2,z_2) \in E^h$ and $t \in (0,1)$, and let $(x,z) := t(x_1,z_1) + (1-t)(x_2,z_2)$. Since $h(z_i) < \infty$ for $i = 1,2$, we must have $h(z) \leq th(z_1) + (1-t)h(z_2) < \infty$. Moreover, it follows from the definition of E^h that there exist $\lambda_1, \lambda_2 \in (0,\infty)$ and $y_1, y_2 \in E$ such that $\lambda_i \geq h(z_i)$ and $x_i = \lambda_i y_i$ for each $i = 1,2$. Let $\lambda := t\lambda_1 + (1-t)\lambda_2 \in (0,\infty)$ and observe that

$$x' := x/\lambda = \frac{t\lambda_1}{\lambda} y_1 + \frac{(1-t)\lambda_2}{\lambda} y_2 \in [y_1, y_2] \subseteq E.$$

Thus, if $h(z) = 0$, then $x = \lambda x' \in \bigcup_{\lambda>0} \lambda E$. Otherwise, if $h(z) \in (0,\infty)$, then

$$\lambda' := \frac{\lambda}{h(z)} \geq \frac{th(z_1) + (1-t)h(z_2)}{h(tz_1 + (1-t)z_2)} \geq 1,$$

so $x/h(z) = \lambda' x' \in \lambda' E \subseteq E$. In both cases, we deduce that $(x,z) \in E^h$, and this establishes the convexity of E^h.

Henceforth, suppose that E is closed and $(0,\infty)^d = \bigcup_{\lambda>0} \lambda E$. It follows from these assumptions that $0 \notin E$ and moreover that for each $x \in (0,\infty)^d$, there exists $\alpha_x \in (0,\infty)$ such that $R_x := E \cap \{ax : a \geq 0\} = \{ax : a \geq \alpha_x\}$. Thus, $\tau_E(x) = \max\{\lambda > 0 : x/\lambda \in E\} = 1/\alpha_x$, and it is clear that $\tau_E(\lambda x) = \lambda\tau_E(x)$ for all $\lambda \in (0,\infty)$. Now if $x \notin E$, then $x \notin R_x$, so $\tau_E(x) < 1$. On the other hand, if $x \in \operatorname{Int} E$, then there exists $\delta > 0$ such that $(1-\delta)x \in E$, so $\tau_E(x) > 1$. Otherwise, if $x \in \partial E$, then by the supporting hyperplane theorem (Schneider, 2014, Theorem 1.3.2), there exists an open half-space H^+ such that $x \in \partial H^+$ and $H^+ \cap E = \emptyset$. Note that we cannot have $R_x \subseteq \partial H^+$; indeed, this would imply that $0 \in \partial H^+$, and since there exists $\eta > 0$ such that $B(x,\eta) \subseteq (0,\infty)^d$, it would then follow that $H^+ \cap (0,\infty)^d$ is a non-empty cone that is disjoint from E. But this contradicts the assumption that $(0,\infty)^d = \bigcup_{\lambda>0} \lambda E$, so it is indeed the case that $R_x \nsubseteq \partial H^+$, as claimed. We conclude that $R_x \cap \partial H^+ = \{x\}$ and hence that $\tau_E(x) = 1$.

In summary, for $\lambda \in (0,\infty)$, we have $\tau_E(x) = \lambda\tau_E(x/\lambda) \geq \lambda$ if and only if $x/\lambda \in E$, and $\tau_E(x) = \lambda\tau_E(x/\lambda) > \lambda$ if and only if $x/\lambda \in \operatorname{Int} E$. In other words, $\tau_E^{-1}\big((\lambda,\infty)\big) = \lambda \operatorname{Int} E$ and $\tau_E^{-1}\big((-\infty,\lambda)\big) = (\lambda E)^c$ for each $\lambda > 0$, and since these sets are all open, we conclude that τ_E is continuous on $(0,\infty)^d$. Moreover, we see that $\partial E \cap \lambda E = \emptyset$ for all $\lambda > 1$, which yields the final assertion of (i).

For (ii), observe that if $h(z) = 0$, then $\tau_E(x) \geq h(z) = 0$ for all $x \in (0,\infty)^d = \bigcup_{\lambda>0} \lambda E$. On the other hand, if $h(z) \in (0,\infty)$, then (i) implies that $\tau_E(x) \geq h(z)$ if and only if $x/h(z) \in E$. We conclude that $E^h = \{(x,z) \in (0,\infty)^d \times (0,\infty) : \tau_E(x) \geq h(z)\}$, as required.

Suppose further that h is convex, decreasing and lower semi-continuous, and that $h(x) \nearrow \infty$ as $x \searrow 0$. Now for $c \in [0,\infty)$, let $I_c := \{z \in [0,\infty) : h(z) \leq c\}$ and note that either $I_c = \emptyset$, in which case $h^{-1}(c) = \infty$, or $I_c = [z',\infty)$ for some $z' \in (0,\infty)$, in which case $h^{-1}(c) = z'$. For $z, c \in [0,\infty)$, this shows that $h(z) \leq c$ if and only if $h^{-1}(c) \leq z$; in other words, $(z,c) \in [0,\infty)^2$ lies in the epigraph of h if and only if (c,z) lies in the epigraph of h^{-1}. Since h is convex and lower semi-continuous, the epigraph of h is closed and convex (Rockafellar, 1997, Theorem 7.1), so the same is true of the epigraph of h^{-1}. This in turn implies that h^{-1} is convex and lower semi-continuous. Moreover, since h is decreasing, the same is true of h^{-1}. This yields (iii).

For (iv), we deduce from (ii) and (iii) that

$$E^h = \{(x,z) \in (0,\infty)^{d+1} : \tau_E(x) \geq h(z)\} = \{(x,z) \in (0,\infty)^d \times \mathbb{R} : z \geq (h^{-1} \circ \tau_E)(x)\},$$

where we have used the fact that $h^{-1}(c) > 0$ for all $c \in [0,\infty)$ to obtain the second equality. Thus, $h^{-1} \circ \tau_E$ is a convex function whose epigraph is E^h, and if $h(z) \in (0,\infty)$ for all $z \in (0,\infty)$, then it follows from (i) that

$$\{x \in (0,\infty)^d : z \geq (h^{-1} \circ \tau_E)(x)\} = \{x \in (0,\infty)^d : \tau_E(x) \geq h(z)\} = h(z) \cdot E$$

is closed for all $z \in (0,\infty)$. Together with Rockafellar (1997, Theorem 7.1), this implies that $h^{-1} \circ \tau_E$ is lower semi-continuous and E^h is closed, as required.

Finally, if $(x,z) \in E^h$ and $\lambda \geq 1$, then $\tau_E(x) \geq h(z) \geq h(\lambda z)/\lambda$ by (ii) and the fact that h is decreasing, so it follows from (ii) that $\lambda(x,z) \in E^h$. Also, for a fixed $(x,z) \in (0,\infty)^{d+1}$, note that since $h(tz)/t \to 0$ as $t \to \infty$ if h is not identically ∞, there exists $\lambda > 0$ such that $h(\lambda z)/\lambda \leq \tau_E(x)$. We deduce from (ii) that $\lambda(x,z) \in E^h$, as claimed in (v). $\square$

Lemma 2.7.21. *There exists $\alpha_d > 0$, depending only on $d \in \mathbb{N}$, such that for every $\eta \in (0, 2^{-d}]$, we can construct a $G_R(Q)$-invariant polytope $P_\eta \equiv P_{d,\eta} \subseteq J_{d,\eta} \equiv J_\eta$ with the following properties:*

(i) P_η has at most $\alpha_d \log^{d-1}(1/\eta)$ vertices and $\mu_d(Q \setminus P_\eta) \leq \alpha_d\, \mu_d(Q \setminus J_\eta)$.

(ii) If $0 < \eta < \tilde{\eta} \leq 2^{-d}$, then $P_{\tilde{\eta}} \subsetneqq P_\eta$, and the regions $Q \setminus \operatorname{Int} P_\eta$ and $P_\eta \setminus \operatorname{Int} P_{\tilde{\eta}}$ can each be expressed as the union of at most $\alpha_d \log^{d-1}(1/\eta)$ d-simplices with pairwise disjoint interiors.

(iii) $\tilde{P}_\eta \equiv \tilde{P}_{d,\eta} := Q^\triangle \cap P_{d,\eta}$ is a polytope and $\mu_d(Q^\triangle \setminus \tilde{P}_\eta) \leq \alpha_d\, \mu_d(Q^\triangle \setminus J_\eta)$, where $Q^\triangle$ is defined as in Lemma 2.7.19.

(iv) If $0 < \eta < \tilde{\eta} \leq (d+1)^{-d}$, then $\tilde{P}_{\tilde{\eta}} \subsetneqq \tilde{P}_\eta$, and the regions $Q^\triangle \setminus \operatorname{Int} \tilde{P}_\eta$ and $\tilde{P}_\eta \setminus \operatorname{Int} \tilde{P}_{\tilde{\eta}}$ can each be expressed as the union of at most $\alpha_d \log^{d-1}(1/\eta)$ d-simplices with pairwise disjoint interiors.

A key feature of this result is that the bounds on the number of simplices in (ii) and (iv) have a polylogarithmic (rather than polynomial) dependence on η^{-1}. The proof below is constructive and 'bare-hands' in that it does not appeal to the general theory of polytopal approximations to compact, convex sets. It is instructive to compare our conclusions with what could be obtained by directly applying an off-the-shelf result such as Lemma 2.8.3 in Section 2.8.1, or Gordon et al. (1995, Theorem 3), which states that for any $K \in \mathcal{K}^b$ and $\zeta > 0$, there exists a polytope $P \subseteq K$ with $\lesssim_d \zeta^{-(d-1)/2}$ vertices such that $\mu_d(K \setminus P) \leq \zeta \mu_d(K)$. In (i), we seek a polytope $P \subseteq J_\eta$ such that $\mu_d(Q \setminus P) \leq \alpha_d\, \mu_d(Q \setminus J_\eta)$, and in view of Lemma 2.7.17(iii), the requirement is that

$$\mu_d(J_\eta \setminus P) \leq (\alpha_d - 1)\, \mu_d(Q \setminus J_\eta) \lesssim_d \eta \log^{d-1}(1/\eta) \lesssim_d \eta \log^{d-1}(1/\eta)\, \mu_d(J_\eta),$$

at least when $\eta \leq 2^{-(d+1)}$. It follows from Gordon et al. (1995, Theorem 3) that there exists a suitable polytope P with $\lesssim_d \{\eta \log^{d-1}(1/\eta)\}^{-(d-1)/2}$ vertices, but this bound is much weaker than what is claimed in (i). Similarly, the bounds of order $\log^{d-1}(1/\eta)$ in (ii) and (iv) do not follow straightforwardly from general schemes for approximating and subdividing the region between two nested convex sets or polytopes (cf. Lee, 2004, page 390).

Instead, we exploit the special structure of the regions J_η and A_η defined in Lemma 2.7.17. In particular, the scaling property in Lemma 2.7.17(i) implies that $[0,1/2]^d \cap J_\eta = [0,1/2]^d \cap A_\eta = \eta^{1/d}\left([0,\eta^{-1/d}/2]^d \cap A_1\right)$. In the proof, we aim to construct a set $E \equiv E_d \subseteq A_{d,1} \equiv A_1$ such that $[0,\eta^{-1/d}/2]^d \cap E$ is a polytope satisfying $\mu_d([0,\eta^{-1/d}/2]^d \setminus E) \lesssim_d \mu_d([0,\eta^{-1/d}/2]^d \setminus A_1)$ for all $\eta > 0$. It turns out that this can be achieved whilst also ensuring that $[0,\eta^{-1/d}/2]^d \cap E$ has $\lesssim_d \log^{d-1}(1/\eta)$

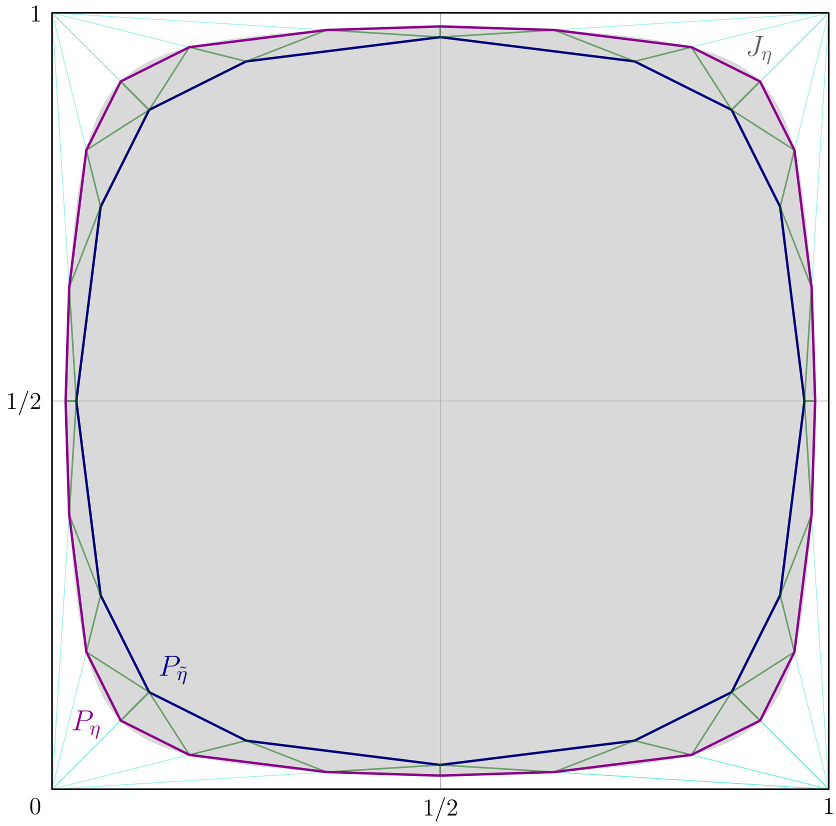

Figure 2.6: Diagram of the nested sets $J_\eta \supseteq P_\eta \supseteq P_{\tilde\eta}$ in Lemma 2.7.21 for $0 < \eta < \tilde\eta \leq 2^{-d}$ when $d = 2$. The grey shaded region is J_η, and the boundaries of P_η and $P_{\tilde\eta}$ are outlined in purple and blue respectively. The x_1-coordinates of the vertices of P_η in $[0, 1/2)^2$ take the form $2^k\eta^{1/2}$, where $k \in \mathbb{Z}$. The green line segments indicate a triangulation of $P_\eta \setminus \operatorname{Int} P_{\tilde\eta}$ that is constructed using a scaling argument, which we illustrate using faint blue line segments; see properties (iv) and (ix) in the proof.

vertices in $[0, \eta^{-1/d}/2)^d$. Intuitively, the reason for this is that the boundary of A_1 becomes much 'flatter' away from the origin, as can be seen in Figures 2.4 and 2.6. This means that the volume bound above can be satisfied by an approximating polytope whose vertices are spread much more diffusely over the boundary of A_1 in regions further away from the origin.

Returning to the original domain $[0, 1/2]^d$, we scale E to get $L_\eta := \eta^{1/d}E \subseteq \eta^{1/d}A_1 = A_\eta$, so that $\mu_d([0, 1/2]^d \cap L_\eta) \lesssim_d \mu_d([0, 1/2]^d \cap J_\eta)$. The polytope P_η is then constructed by applying the isometries in $G_R(Q)$ to $[0, 1/2]^d \cap L_\eta$. By elucidating the facial structure of E and scaling E as above, we proceed to obtain simplicial decompositions of $Q \setminus \operatorname{Int} P_\eta$ and $P_\eta \setminus \operatorname{Int} P_{\tilde\eta}$ that satisfy the conditions of (ii).

Proof of Lemma 2.7.21. Throughout, for $d \in \mathbb{N}$, we identify $\mathbb{R}^d$ and $\mathbb{Z}^d$ with $\mathbb{R}^{d-1} \times \mathbb{R}$ and $\mathbb{Z}^{d-1} \times \mathbb{Z}$ respectively. First, we will show by induction on d that for all $d \in \mathbb{N}$ and $\eta > 0$, there exists a closed, convex set $L_\eta \equiv L_{d,\eta}$ with the following properties:

(i) $L_{d,\eta}$ is the epigraph of a continuous, convex function $g_\eta : (0, \infty)^{d-1} \to (0, \infty)$ with the property that $g_\eta(u) \geq s_\eta(u) := \eta \prod_{j=1}^{d-1} u_j^{-1}$ for all $u \in \mathbb{R}^d$, and $\partial L_{d,\eta} = \{(x, g_\eta(x)) : x \in (0, \infty)^{d-1}\}$.

(ii) $\lambda L_{d,\eta} \subseteq L_{d,\eta} \subseteq A_{d,\eta}$ for all $\lambda \geq 1$ and $(0, \infty)^d = \bigcup_{\lambda > 0} \lambda L_{d,\eta}$.

(iii) If $(x_1, \ldots, x_d) \in L_{d,\eta}$, then $(x_1', \ldots, x_d') \in L_{d,\eta}$ whenever $x_j' \geq x_j$ for all $1 \leq j \leq d$. Also, if $(x_1, \ldots, x_d) \in \operatorname{Int} L_{d,\eta}$, then $(x_1', \ldots, x_d') \in \operatorname{Int} L_{d,\eta}$ whenever $x_j' \geq x_j$ for all j.

(iv) $L_{d,\eta} = \eta^{1/d} L_{d,1} =: \eta^{1/d} E_d$ and $(\eta^{1/d}, \ldots, \eta^{1/d}) \in \mathbb{R}^d$ lies in $L_{d,\eta}$. If $\tilde\eta > \eta$, then $L_{d,\tilde\eta} = (\tilde\eta/\eta)^{1/d} L_{d,\eta} \subsetneqq L_{d,\eta}$. Moreover, $[0, 1/2]^d \cap L_{d,\eta}$ is non-empty if and only if $\eta \in (0, 2^{-d}]$, and $[0, 1/2]^d \cap \operatorname{Int} L_{d,\eta}$ is non-empty if and only if $\eta \in (0, 2^{-d})$.

(v) Every facet of $L_{d,\eta}$ is a $(d-1)$-dimensional polytope and every $x \in \partial L_{d,\eta}$ lies in some facet. More precisely, if $d \geq 2$ and F is a facet of $L_{d,\eta}$, then there exists $m' = (m, j) \in \mathbb{Z}^{d-2} \times \mathbb{Z} \equiv \mathbb{Z}^{d-1}$ such that $F = F_{\eta,m'} := \{(\lambda x, g_\eta(\lambda x)) : x \in G_m,\, \lambda \in [w_{\eta,j}, w_{\eta,j-1}]\}$, where G_m is a corresponding facet of E_{d-1} and $w_{\eta,k} \equiv w_{d,\eta,k} := 2^{-k}\eta^{1/d}$ for $k \in \mathbb{Z}$. Moreover, $F_{\eta,m'} = \eta^{1/d} F_{1,m'} =: G_{m'}$ for all $m' \in \mathbb{Z}^{d-1}$, and if $(x_1, \ldots, x_d) \in F_{\eta,m'}$, then $x_d \in [z_{\eta,j-1}, z_{\eta,j}]$, where $z_{\eta,k} \equiv z_{d,\eta,k} := 2^{(d-1)k}\eta^{1/d}$ for $k \in \mathbb{Z}$.

We will then show by induction on d that for all $d \in \mathbb{N}$, there exists $\alpha'_d > 0$, depending only on d, such that the following hold for all $\eta \in (0, 2^{-d}]$:

(vi) $P_\eta \equiv P_{d,\eta} := \bigcap_{g \in G_R(Q)} g(L_{d,\eta} \cap Q)$ is non-empty and $G_R(Q)$-invariant, and $P_{d,\eta} \subseteq J_{d,\eta}$.

(vii) $[0, 1/2]^d \cap P_{d,\eta} = [0, 1/2]^d \cap L_{d,\eta}$ and $[0, 1/2]^d \cap \operatorname{Int} P_{d,\eta} = [0, 1/2]^d \cap \operatorname{Int} L_{d,\eta}$. Moreover, $\mu_d([0, 1/2]^d \setminus P_{d,\eta}) \leq \alpha'_d\, \mu_d([0, 1/2]^d \setminus J_{d,\eta})$.

(viii) $P_{d,\eta}$ is a polytope with at most $\alpha'_d \log^{d-1}(1/\eta)$ vertices.

(ix) If $0 < \eta < \tilde{\eta} \leq 2^{-d}$, then $[0, 1/2]^d \setminus \operatorname{Int} P_{d,\eta}$ and $[0, 1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})$ can each be triangulated into at most $\alpha'_d \log^{d-1}(1/\eta)$ d-simplices, in such a way that for any d-simplex S in the triangulation of $[0, 1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})$, there exists $m' \in \mathbb{Z}^{d-1}$ such that $S \subseteq \bigcup_{\lambda \in [1, (\tilde{\eta}/\eta)^{1/d}]} \lambda F_{\eta,m'} = \bigcup_{\lambda \in [\eta^{1/d},\, \tilde{\eta}^{1/d}]} \lambda G_{m'}$.

In view of the $G_R(Q)$-invariance of P_η, these final four assertions imply parts (i) and (ii) of the desired result. We will address parts (iii) and (iv) of the lemma at the end of the proof.

When $d = 1$, we can take $L_{1,\eta} := A_{1,\eta} = [\eta, \infty)$ and $P_{1,\eta} := J_{1,\eta} = [\eta, 1 - \eta]$ for each $\eta \in (0, 1/2]$, which trivially have the desired properties. Note that $L_{1,\eta}$ has a single facet $F_{\eta,\varnothing} := \{\eta\}$, where we write $\varnothing$ for the empty tuple. Next, for fixed $d \geq 2$ and $\eta > 0$, let $\overline{h}_\eta(z) \equiv \overline{h}_{d,\eta}(z) := (\eta/z)^{1/(d-1)}$ for each $z \in (0, \infty)$ and let $h_\eta \equiv h_{d,\eta} \colon (0, \infty) \to (0, \infty)$ be the piecewise affine function that is linear on each of the intervals $[z_{\eta,j-1}, z_{\eta,j}]$ and satisfies $h_\eta(z_{\eta,j}) = w_{\eta,j} = \overline{h}_\eta(z_{\eta,j})$ for all $j \in \mathbb{Z}$. Then h_η is a strictly decreasing, convex bijection whose inverse $h_\eta^{-1} \colon (0, \infty) \to (0, \infty)$ is also piecewise affine. Indeed, for $j \in \mathbb{Z}$, let $t_{\eta,j}$ be the (unique) affine function that satisfies $t_{\eta,j}(w_{\eta,j}) = z_{\eta,j}$ and $t_{\eta,j}(w_{\eta,j-1}) = z_{\eta,j-1}$, and observe that $h_\eta^{-1}(w) \geq t_{\eta,j}(w)$ for all $w \in (0, \infty)$, with equality if and only if $w \in [w_{\eta,j}, w_{\eta,j-1}]$.

We now verify that $\overline{h}_\eta \leq h_\eta \leq \gamma_d \overline{h}_\eta$ for some $\gamma_d > 0$ that depends only on d. Indeed, if $z = \lambda z_{\eta,j} \in [z_{\eta,j}, z_{\eta,j+1}]$ for some $j \in \mathbb{Z}$ and $\lambda \in [1, 2^{d-1}]$, then

$$\frac{h_\eta(z)}{\overline{h}_\eta(z)} = \frac{\bigl\{1 - (\lambda - 1)/(2^d - 2)\bigr\}\, h_\eta(z_{\eta,j})}{\lambda^{-1/(d-1)}\, \overline{h}_\eta(z_{\eta,j})} = \frac{(2^d - \lambda - 1)\, \lambda^{1/(d-1)}}{2^d - 2}\,, \tag{2.7.23}$$

which is independent of j and attains its maximum value when $\lambda = (2^d - 1)/d$. Also, it is easy to see that $h_\eta(z) = \eta^{1/d} h_1(z/\eta^{1/d})$ and $h_\eta^{-1}(w) = \eta^{1/d} h_1^{-1}(w/\eta^{1/d})$ for all $z, w \in (0, \infty)$. Since h_1 is strictly decreasing, it follows that $h_\eta < h_{\tilde{\eta}}$ whenever $0 < \eta < \tilde{\eta}$.

Using the notation of Lemma 2.7.20, we claim that $L_{d,\eta} := (E_{d-1})^{h_\eta}$ has the required properties (i)–(v), where $E_{d-1} \equiv L_{d-1,1}$.

Properties (i) and (ii). By part (ii) of the inductive hypothesis and Lemma 2.7.20(iv), it follows that $L_{d,\eta}$ is closed and convex, and that $g_\eta := h_\eta^{-1} \circ \tau_{E_{d-1}}$ is a convex function whose epigraph is $L_{d,\eta}$. Since h_η^{-1} and $\tau_{E_{d-1}}$ are continuous, it follows that g_η is continuous and hence that $\partial L_{d,\eta} = \{(x, g_\eta(x)) : x \in (0, \infty)^{d-1}\}$. In addition, Lemma 2.7.20(v) implies that $\lambda L_{d,\eta} \subseteq L_{d,\eta}$ for all

$\lambda \geq 1$ and $(0,\infty)^d = \bigcup_{\lambda>0} \lambda L_{d,\eta}$. Now for each $z \in (0,\infty)$, observe that

$$\begin{aligned} L_{d,\eta} \cap \bigl((0,\infty)^{d-1} \times \{z\}\bigr) &= (h_\eta(z) \cdot E_{d-1}) \times \{z\} && (2.7.24)\\ &\subseteq (h_\eta(z) \cdot A_{d-1,1}) \times \{z\} \subseteq (\overline{h}_\eta(z) \cdot A_{d-1,1}) \times \{z\} && (2.7.25)\\ &= A_{d-1,\,\eta/z} \times \{z\} = A_{d,\eta} \cap \bigl((0,\infty)^{d-1} \times \{z\}\bigr); \end{aligned}$$

indeed, the first inclusion in (2.7.25) follows from part (ii) of the inductive hypothesis, which ensures that $E_{d-1} = L_{d-1,1} \subseteq A_{d-1,1}$, and the second inclusion follows from the definition of $A_{d-1,1}$ and the fact that $\overline{h}_\eta \leq h_\eta$. This shows that $L_{d,\eta} \subseteq A_{d,\eta}$.

Property (iii). Now fix $(x,z) \in L_{d,\eta}$ and let $x' \in (0,\infty)^{d-1}$ be such that $x'_j \geq x_j$ for all $1 \leq j \leq d-1$. It follows from parts (ii) and (iii) of the inductive hypothesis that $\tau_{E_{d-1}}(x') \geq \tau_{E_{d-1}}(x)$. Since $L_{d,\eta} = \{(x,z) : x \in (0,\infty)^d,\ z \geq g_\eta(x)\}$, we see that if $z' \geq z$, then

$$z' \geq z \geq g_\eta(x) = (h_\eta^{-1} \circ \tau_{E_{d-1}})(x) \geq (h_\eta^{-1} \circ \tau_{E_{d-1}})(x') = g_\eta(x'),$$

so $(x',z') \in L_{d,\eta}$. This yields the first assertion of (iii). Since $\operatorname{Int} L_{d,\eta} = \{(x,z) : x \in (0,\infty)^d,\ z > g_\eta(x)\}$ by property (i), we can argue similarly to obtain the corresponding conclusion when $L_{d,\eta}$ is replaced by $\operatorname{Int} L_{d,\eta}$ throughout.

Property (iv). Note that $(x,z) \in (0,\infty)^d$ lies in $L_{d,\eta}$ if and only if $(\eta^{-1/d}x)/h_1(\eta^{-1/d}z) = x/h_\eta(z) \in E_{d-1}$, i.e. $\eta^{-1/d}(x,z) \in L_{d,1}$. Thus, if $\tilde{\eta} > \eta$, then $L_{d,\tilde{\eta}} = \tilde{\eta}^{1/d} L_{d,1} \equiv \tilde{\eta}^{1/d} E_d = (\tilde{\eta}/\eta)^{1/d} L_{d,\eta} \subsetneq L_{d,\eta}$ by property (ii) and Lemma 2.7.20(i). Moreover, $h_\eta(\eta^{1/d}) = \overline{h}_\eta(\eta^{1/d}) = \eta^{1/d}$, and part (iv) of the inductive hypothesis asserts that E_{d-1} contains $(1,\dots,1) \in \mathbb{R}^{d-1}$, so we deduce from (2.7.24) that $L_{d,\eta}$ contains $(\eta^{1/d},\dots,\eta^{1/d}) \in \mathbb{R}^d$. It follows from this and property (iii) that $\tau_{E_d}(x) \leq \tau_{E_d}((1/2,\dots,1/2)) = 1/2$ for all $x \in [0,1/2]^d$. Together with property (ii) and Lemma 2.7.20(i), this shows that $[0,1/2]^d \cap L_{d,\eta} = \{x \in [0,1/2]^d : \tau_{E_{d-1}}(x) \geq \eta^{1/d}\}$ is non-empty if and only if $\eta \in (0,2^{-d}]$, and that $[0,1/2]^d \cap \operatorname{Int} L_{d,\eta} = \{x \in [0,1/2]^d : \tau_{E_{d-1}}(x) > \eta^{1/d}\}$ is non-empty if and only if $\eta \in (0,2^{-d})$.

Property (v). Next, we investigate the facial structure of $L_{d,\eta}$. By part (v) of the inductive hypothesis, every facet of E_{d-1} is a polytope of the form $G_m \equiv F_{1,m}$ for some $m \in \mathbb{Z}^{d-2}$. For each such m, let $\theta_m \in \mathbb{R}^{d-1}$ be such that $H_m := \{u \in \mathbb{R}^{d-1} : \theta_m^\top u = 1\}$ is a supporting hyperplane to E_{d-1} with $E_{d-1} \cap H_m = G_m$. Since H_m is disjoint from $\operatorname{Int} E_{d-1}$ and $x \in (\theta_m^\top x)\,H_m$ for all $x \in (0,\infty)^{d-1}$, it follows from Lemma 2.7.20(i) that $\tau_{E_{d-1}}(x) \leq \theta_m^\top x$ for all $x \in (0,\infty)^{d-1}$, with equality if and only if $x \in (\theta_m^\top x)\,(E_{d-1} \cap H_m) = (\theta_m^\top x)\,G_m$, i.e. $x \in \bigcup_{\lambda>0} \lambda G_m$. Therefore,

$$g_\eta(x) = (h_\eta^{-1} \circ \tau_{E_{d-1}})(x) \geq h_\eta^{-1}(\theta_m^\top x) \geq t_{\eta,j}(\theta_m^\top x) \tag{2.7.26}$$

for all $x \in (0,\infty)^{d-1}$, with equality if and only if $x \in D_{m,j} := \bigcup_{\lambda \in [w_{\eta,j},\,w_{\eta,j-1}]} \lambda G_m$.

Observe that $D_{m,j}$ is a $(d-1)$-dimensional polytope; indeed, writing V_m for the (finite) set of extreme points of the polytope G_m, we see that $V_{m,j} := \{\lambda u : \lambda \in \{w_{\eta,j},\, w_{\eta,j-1}\},\ u \in V_m\}$ is the set of extreme points of $D_{m,j}$. Setting $m' = (m,j) \in \mathbb{Z}^{d-2} \times \mathbb{Z} \equiv \mathbb{Z}^{d-1}$, we deduce from (2.7.26) that the restriction of g_η to $D_{m,j}$ is an affine function $x \mapsto t_{\eta,j}(\theta_m^\top x)$, and moreover that $L_{d,\eta}$ is contained within the closed half-space $H_{\eta,m'}^+ := \{(x,z) \in \mathbb{R}^d : z \geq t_{\eta,j}(\theta_m^\top x)\}$. It follows that $H_{\eta,m'} := \partial H_{\eta,m'}^+ = \{(x, t_{\eta,j}(\theta_m^\top x)) : x \in \mathbb{R}^{d-1}\} \subseteq \mathbb{R}^d$ is a supporting hyperplane to $L_{d,\eta}$ and that

$$F_{\eta,m'} := L_{d,\eta} \cap H_{\eta,m'} = \{(x, g_\eta(x)) : x \in D_{m,j}\} = \{(x, t_{\eta,j}(\theta_m^\top x)) : x \in D_{m,j}\} \subseteq \partial L_{d,\eta}$$

is a facet of $L_{d,\eta}$. In addition, the set of extreme points of $F_{\eta,m'}$ is $V_{\eta,m'} := \{(x, g_\eta(x)) : x \in V_{m,j}\}$, so $F_{\eta,m'}$ is also a $(d-1)$-dimensional polytope.

Since $g_\eta(x) = (h_\eta^{-1} \circ \tau_{E_{d-1}})(x) = \eta^{1/d} h_\eta^{-1}(\tau_{E_{d-1}}(x)/\eta^{1/d}) = \eta^{1/d} g_1(x/\eta^{1/d})$ for all $x \in (0,\infty)^{d-1}$, it follows that $x' \in F_{\eta,m'}$ if and only if there exists $\lambda' \in [2^{-j}, 2^{-j+1}] = [w_{1,j}, w_{1,j-1}]$ and $x \in G_m$ such that $x' = (\eta^{1/d}\lambda' x, g_\eta(\eta^{1/d}\lambda' x)) = \eta^{1/d}(\lambda' x, g_1(\lambda' x))$. This shows that $F_{\eta,m'} = \eta^{1/d} F_{1,m'} \equiv G_{m'}$. Moreover, since $\theta_m^\top x = \tau_{E_{d-1}}(x) \in [w_{\eta,j}, w_{\eta,j-1}]$ for all $x \in D_{m,j}$, we have $g_\eta(x) = t_{\eta,j}(\theta_m^\top x) \in [h_\eta^{-1}(w_{\eta,j-1}), h_\eta^{-1}(w_{\eta,j})] = [z_{\eta,j-1}, z_{\eta,j}]$ for all $x \in D_{m,j}$.

By applying parts (ii) and (v) of the inductive hypothesis, we find that

$$(0,\infty)^{d-1} = \bigcup_{\lambda>0} \lambda\,\partial E_{d-1} = \bigcup_{m\in\mathbb{Z}^{d-2}} \bigcup_{j\in\mathbb{Z}} \bigcup_{\lambda\in[w_{\eta,j}, w_{\eta,j-1}]} \lambda G_m = \bigcup_{(m,j)\in\mathbb{Z}^{d-2}\times\mathbb{Z}} D_{m,j}.$$

Thus, for every $x' = (x, g_\eta(x)) \in \partial L_{d,\eta}$, there exists $m' = (m,j) \in \mathbb{Z}^{d-1}$ such that $x \in D_{m,j}$, so that $x' \in F_{\eta,m'}$. Furthermore, if F is an arbitrary facet of $L_{d,\eta}$, then there exist $m' = (m,j) \in \mathbb{Z}^{d-1}$ and $x \in \operatorname{Int} D_{m,j}$ such that $(x, g_\eta(x)) \in \operatorname{relint} F \subseteq \partial L_{d,\eta}$. But since $(x, g_\eta(x)) \in \operatorname{relint} F_{\eta,m'}$, it follows that $(\operatorname{relint} F) \cap (\operatorname{relint} F_{\eta,m'}) \neq \emptyset$, whence $F = F_{\eta,m'}$ by Schneider (2014, Theorem 2.1.2).

Having established properties (i)–(v) of $L_{d,\eta}$, we now verify that $P_{d,\eta} = \bigcap_{g\in G_R(Q)} g(L_{d,\eta} \cap Q)$ has the required properties (vi)–(ix).

Property (vi). Since $L_{d,\eta} \cap Q$ is compact and convex, it follows that $P_{d,\eta}$ is a compact, convex and $G_R(Q)$-invariant subset of Q. Moreover, we have

$$P_{d,\eta} = \bigcap_{g\in G_R(Q)} g(L_{d,\eta} \cap Q) \subseteq \bigcap_{g\in G_R(Q)} g(A_{d,\eta} \cap Q) = J_{d,\eta}$$

by property (ii) of $L_{d,\eta}$ and Lemma 2.7.17(ii).

Property (vii). Recalling the definition of the function $M : Q \to [0,1/2]^d$ from the paragraph before Lemma 2.7.17, we deduce from property (iii) of $L_{d,\eta}$ that for $x \in Q$, we have $g(x) \in L_{d,\eta}$ for all $g \in G_R(Q)$ if and only if $M(x) \in L_{d,\eta}$. Thus, it follows as in the proof of Lemma 2.7.17(ii) that $P_{d,\eta} = \{x \in Q : M(x) \in L_{d,\eta}\}$ and hence that $[0,1/2]^d \cap P_{d,\eta} = [0,1/2]^d \cap L_{d,\eta}$. By a similar argument based on property (iii), we deduce that $\operatorname{Int} P_{d,\eta} = \{x \in Q : M(x) \in \operatorname{Int} L_{d,\eta}\}$ and hence that $[0,1/2]^d \cap \operatorname{Int} P_{d,\eta} = [0,1/2]^d \cap \operatorname{Int} L_{d,\eta}$. Turning to the last assertion of (vii), it suffices to show that there exists $\alpha_d'' > 0$, depending only on d, such that

$$\mu_{d-1}\big(([0,1/2]^{d-1} \times \{z\}) \setminus P_{d,\eta}\big) \le \alpha_d''\, \mu_{d-1}\big(([0,1/2]^{d-1} \times \{z\}) \setminus J_{d,\eta}\big) \tag{2.7.27}$$

for all $z \in [0,1/2]$, since we can then integrate this inequality with respect to z to conclude that $\mu_d([0,1/2]^d \setminus P_{d,\eta}) \le \alpha_d''\, \mu_d([0,1/2]^d \setminus J_{d,\eta})$. To this end, fix $z \in [0,1/2]$ and observe that by (2.7.24) and property (vi), the left hand side of (2.7.27) is equal to

$$\begin{aligned}\mu_{d-1}\big(([0,1/2]^{d-1} \times \{z\}) \setminus L_{d,\eta}\big) &= \mu_{d-1}\big([0,1/2]^{d-1} \setminus (h_\eta(z) \cdot E_{d-1})\big) \\ &= \mu_{d-1}\big([0,1/2]^{d-1} \setminus L_{d-1,\, h_\eta(z)^{d-1}}\big).\end{aligned}$$

By applying part (vii) of the inductive hypothesis, Lemma 2.7.17(iii), (2.7.23) and Lemma 2.7.17(i) in that order, we find that

$$
\begin{aligned}
\mu_{d-1}([0,1/2]^{d-1} \setminus L_{d-1,\,h_\eta(z)^{d-1}}) &= \mu_{d-1}([0,1/2]^{d-1} \setminus P_{d-1,\,h_\eta(z)^{d-1}}) \\
&\leq \alpha'_{d-1}\, \mu_{d-1}([0,1/2]^{d-1} \setminus J_{d-1,\,h_\eta(z)^{d-1}}) \\
&\leq \alpha'_{d-1}\, \{h_\eta(z)/\overline{h}_\eta(z)\}^{d-1}\, \mu_{d-1}([0,1/2]^{d-1} \setminus J_{d-1,\overline{h}_\eta(z)^{d-1}}) \\
&\leq \alpha'_{d-1}\, \gamma_d^{d-1} \mu_{d-1}([0,1/2]^{d-1} \setminus A_{d-1,\overline{h}_\eta(z)^{d-1}}) \\
&= \alpha'_{d-1}\gamma_d^{d-1}\, \mu_{d-1}(([0,1/2]^{d-1} \times \{z\}) \setminus A_{d,\eta}), \\
&= \alpha'_{d-1}\gamma_d^{d-1}\, \mu_{d-1}(([0,1/2]^{d-1} \times \{z\}) \setminus J_{d,\eta}),
\end{aligned}
$$

which completes the proof of (2.7.27) and hence that of (vii).

Property (viii). In view of properties (iv) and (vii), it suffices to consider $\eta \in (0, 2^{-d}]$, since otherwise $P_{d,\eta} = \emptyset$. Note that for $x \in (0,\infty)^{d-1}$, Lemma 2.7.20(i) implies that $g_\eta(x) = (h_\eta^{-1} \circ \tau_{E_{d-1}})(x) \leq 1/2$ if and only if $\tau_{E_{d-1}}(x) \geq h_\eta(1/2)$. By property (iv), this is the case if and only if $x \in h_\eta(1/2) \cdot E_{d-1} = L_{d-1,\,h_\eta(1/2)^{d-1}}$. In view of property (vii), it follows that

$$
\begin{aligned}
[0,1/2]^d \cap \partial P_{d,\eta} = [0,1/2]^d \cap \partial L_{d,\eta} &= \bigl\{(x, g_\eta(x)) : x \in [0,1/2]^{d-1},\, g_\eta(x) \leq 1/2\bigr\} \\
&= \bigl\{(x, g_\eta(x)) : x \in [0,1/2]^{d-1} \cap L_{d-1,\,h_\eta(1/2)^{d-1}}\bigr\}. \qquad (2.7.28)
\end{aligned}
$$

With the aid of this identity and the inductive hypothesis, we will identify a finite set U' such that $U' \subseteq [0,1/2]^d \cap \partial P_{d,\eta} \subseteq \operatorname{conv} U'$ and $|U'| \lesssim_d \log^{d-1}(1/\eta)$. We will then deduce that $P_{d,\eta}$ is the convex hull of $U := \bigcup_{g \in G_R(Q)} g(U')$ and hence that (viii) holds.

To this end, fix $\eta \in (0, 2^{-d}]$ and let $j_- := \lfloor \log_2(2\eta^{1/d}) \rfloor + 1$ and $j_+ := \lceil \log_2\bigl(\eta^{1/d}/h_\eta(1/2)\bigr) \rceil$, so that j_- is the smallest integer j for which $w_{\eta,j} = 2^{-j}\eta^{1/d} < 1/2$ and j_+ is the smallest integer j for which $w_{\eta,j} \leq h_\eta(1/2)$. Since $h_\eta(1/2) \geq \overline{h}_\eta(1/2) = (2\eta)^{1/(d-1)}$, we have

$$
\begin{aligned}
&j_+ \leq 1 + \log_2\bigl(\eta^{1/d}/h_\eta(1/2)\bigr) \leq 1 + \log_2\bigl(\eta^{1/d}/\overline{h}_\eta(1/2)\bigr) \leq 1 + \tfrac{1}{d(d-1)} \log_2(1/\eta) \quad \text{and} \\
&j_- \geq 1 + \log_2(2\eta^{1/d}) = 2 - \tfrac{1}{d} \log_2(1/\eta),
\end{aligned}
$$

so $j_+ - j_- + 1 \leq \frac{1}{d-1} \log_2(1/\eta) \leq 2\log(1/\eta)$. For $j = j_-, \ldots, j_+$, let $L'_j := L_{d-1,\,\{w_{\eta,j} \vee h_\eta(1/2)\}^{d-1}}$ and $P'_j := P_{d-1,\,\{w_{\eta,j} \vee h_\eta(1/2)\}^{d-1}}$, and for convenience, set $P_{j_- -1} := \emptyset$. Then by property (iv) above, we have $L'_j = L_{d-1,\,w_{\eta,j}^d} = w_{\eta,j} E_{d-1} = 2L'_{j-1}$ for $j = j_- + 1, \ldots, j_+ - 1$ and

$$
L'_{j_+} = L_{d-1,\,h_\eta(1/2)^{d-1}} = h_\eta(1/2) \cdot E_{d-1}.
$$

Recall also that by properties (iii) and (iv) above, we have $\tau_{E_{d-1}}(x) \leq \tau_{E_{d-1}}((1/2,\ldots,1/2)) = 1/2$ for all $x \in [0,1/2]^{d-1}$. Thus, continuing on from (2.7.28) and recalling part (vii) of the inductive hypothesis, we can write

$$
\begin{aligned}
[0,1/2]^{d-1} \cap P'_{j_+} = [0,1/2]^{d-1} \cap L'_{j_+} &= \bigl\{x \in [0,1/2]^{d-1} : h_\eta(1/2) \leq \tau_{E_{d-1}}(x) \leq 1/2\bigr\} \\
&= \textstyle\bigcup_{j=j_-}^{j_+} \bigl\{[0,1/2]^{d-1} \cap (P'_j \setminus \operatorname{Int} P'_{j-1})\bigr\}; \qquad (2.7.29)
\end{aligned}
$$

note in particular that by Lemma 2.7.20(i) and our choice of $j_\pm$, it follows that

$$\begin{aligned}[0,1/2]^{d-1}\cap(P'_j\setminus\operatorname{Int}P'_{j-1})&=[0,1/2]^{d-1}\cap(L'_j\setminus\operatorname{Int}L'_{j-1})\\&=\bigl\{x\in[0,1/2]^{d-1}:\tau_{E_{d-1}}(x)\in[w_{\eta,j}\vee h_\eta(1/2),w_{\eta,j-1}\wedge 1/2]\bigr\}\\&\subseteq[0,1/2]^{d-1}\cap\textstyle\bigcup_{\lambda\in[w_{\eta,j},w_{\eta,j-1}]}\lambda\,\partial E_{d-1}\end{aligned}\tag{2.7.30}$$

for all $j\in\{j_-,\dots,j_+\}$, and moreover that the interiors of these sets are non-empty and pairwise disjoint. Since $2^{-(d-1)}=h_{2^{-d}}(1/2)^{d-1}\geq h_\eta(1/2)^{d-1}\geq\overline{h}_\eta(1/2)^{d-1}=2\eta$, we deduce from part (ix) of the inductive hypothesis and (2.7.30) that the following holds for all $j\in\{j_-,\dots,j_+\}$: the set $[0,1/2]^{d-1}\cap(P'_j\setminus\operatorname{Int}P'_{j-1})$ can be triangulated into at most $\alpha'_{d-1}\log^{d-2}(1/\eta)$ simplices of dimension $d-1$, in such a way that for every constituent simplex S, there exists $m\in\mathbb{Z}^{d-2}$ such that $S\subseteq\bigcup_{[w_{\eta,j},w_{\eta,j-1}]}\lambda G_m=D_{m,j}$.

Recall from (2.7.26) that $g_\eta|_{D_{m,j}}$ is affine on $D_{m,j}$ for all $(m,j)\in\mathbb{Z}^{d-2}\times\mathbb{Z}$. Thus, by the deduction in the previous paragraph and (2.7.29), it follows that there is a triangulation of $[0,1/2]^{d-1}\cap L'_{j_+}$ into $(d-1)$-simplices $S_1,\dots,S_N$, where $N\leq(j_+-j_-+1)\,\alpha'_{d-1}\log^{d-2}(1/\eta)\leq 2\alpha'_{d-1}\log^{d-1}(1/\eta)$ and the restriction of g_η to each S_k is an affine function. For each $1\leq k\leq N$, this implies that $R_k:=\{(x,g_\eta(x)):x\in S_k\}$ is a $(d-1)$-simplex and that there exists $m'\in\mathbb{Z}^{d-1}$ such that $R_k\subseteq F_{\eta,m'}\subseteq\partial L_{d,\eta}$. Writing U_k for the set of vertices of R_k and setting $U':=\bigcup_{k=1}^N U_k$, we deduce from (2.7.28) that

$$U'\subseteq[0,1/2]^d\cap\partial P_{d,\eta}=\textstyle\bigcup_{k=1}^N R_k\subseteq\operatorname{conv}U'.\tag{2.7.31}$$

By applying the (affine) isometries in $G_R(Q)$, we conclude that every $u\in\partial P_{d,\eta}$ lies in the convex hull of $U:=\bigcup_{g\in G_R(Q)}g(U')=\bigcup_{g\in G_R(Q)}\bigcup_{k=1}^N g(U_k)$, and it then follows from the convexity of $P_{d,\eta}$ that $P_{d,\eta}=\operatorname{conv}\partial P_{d,\eta}=\operatorname{conv}U$. Since $|U_k|=d$ for all $1\leq k\leq N$ and $|G_R(Q)|=2^d$, this implies that $P_{d,\eta}$ is a polytope with at most $|U|\leq 2^d\,dN\leq 2^{d+1}\,d\alpha'_{d-1}\log^{d-1}(1/\eta)$ vertices, so the proof of (viii) is complete.

Property (ix). We start by observing that in each of the following cases, the construction from Lee (2004, Section 17.5.1) yields a triangulation of any polytope $K\subseteq\mathbb{R}^d$ of the specified form into d simplices of dimension d, each of which is the convex hull of $d+1$ vertices of K:

(a) $K=S\times[0,1]$, where $S\subseteq\mathbb{R}^{d-1}$ is a $(d-1)$-simplex;

(b) $K=S_h^{\downarrow}:=\{(x,z)\in S\times\mathbb{R}:0\leq z\leq h(x)\}$, where $S\subseteq\mathbb{R}^{d-1}$ is a $(d-1)$-simplex and $h\colon S\to\mathbb{R}$ is an affine function that is strictly positive on S;

(c) $K=\bigcup_{\lambda\in[a,b]}\lambda S$, where $0<a<b$ and $S\subseteq\mathbb{R}^d\setminus\{0\}$ is a $(d-1)$-simplex.

Indeed, it is easily seen that all such polytopes are combinatorially isomorphic in the sense of Henk et al. (2004, Section 16.1.1), so the same explicit construction works in all cases.

We will now triangulate $[0,1/2]^d\setminus\operatorname{Int}P_{d,\eta}$ by 'lifting' an suitable triangulation of $[0,1/2]^{d-1}$ and then applying the fact above. Let $S_1,\dots,S_N$ be the $(d-1)$-simplices that constitute the triangulation of $P'_{j_+}=P_{d-1,\,h_\eta(1/2)^{d-1}}$ obtained in the proof of (viii). By part (ix) of the inductive hypothesis, we can also triangulate $[0,1/2]^{d-1}\setminus\operatorname{Int}P'_{j_+}$ into $(d-1)$-simplices $S_{N+1},\dots,S_{N+M}$, where $M\leq\alpha'_{d-1}\log^{d-2}(1/\eta)$.

Recall now that $\operatorname{Int}L_{d,\eta}=\{(x,z)\in(0,\infty)^d:z>g_\eta(x)\}$ by property (i) above. For $x\in(0,\infty)^{d-1}$, Lemma 2.7.20(i) implies that $g_\eta(x)\leq 1/2$ if and only if $x\in L'_{j_+}$, and $g_\eta(x)<1/2$ if and only if $x\in\operatorname{Int}L'_{j_+}$; see also (2.7.28). Also, by property (vii), we have $[0,1/2]^{d-1}\cap P'_{j_+}=[0,1/2]^{d-1}\cap L'_{j_+}$ and $[0,1/2]^{d-1}\cap\operatorname{Int}P'_{j_+}=[0,1/2]^{d-1}\cap\operatorname{Int}L'_{j_+}$. Therefore, for $x\in[0,1/2]^{d-1}\cap P'_{j_+}$, we have $(x,z)\in[0,1/2]^d\setminus\operatorname{Int}L_{d,\eta}$ if and only if $0\leq z\leq g_\eta(x)$, whereas for $x\in[0,1/2]^{d-1}\setminus\operatorname{Int}P'_{j_+}$, we have

$(x,z) \in [0,1/2]^d \setminus \operatorname{Int} L_{d,\eta}$ for all $z \in [0,1/2]$. Recalling from the paragraph before (2.7.31) that g_η is affine on each of the simplices $S_1,\ldots,S_N$, we deduce that

$$\begin{aligned}[0,1/2]^d \setminus \operatorname{Int} P'_{j_+} = [0,1/2]^d \setminus \operatorname{Int} L'_{j_+} &= \bigl\{(x,z) : x \in [0,1/2]^{d-1} \cap P'_{j_+},\, 0 \leq z \leq g_\eta(x)\bigr\} \cup \\ &\quad \bigl\{(x,z) : x \in [0,1/2]^{d-1} \setminus \operatorname{Int} P'_{j_+},\, z \in [0,1/2]\bigr\} \\ &= \bigl(\textstyle\bigcup_{k=1}^N (S_k)_{g_\eta}^{\downarrow}\bigr) \cup \bigl(\textstyle\bigcup_{m=1}^M S_{N+m} \times [0,1/2]\bigr).\end{aligned}$$

By appealing to cases (a) and (b) of the fact above, we conclude that $[0,1/2]^d \setminus \operatorname{Int} P'_{j_+}$ can be triangulated into $d(N+M) \leq 3d\alpha'_{d-1}\log^{d-1}(1/\eta)$ simplices.

Now if $0 < \eta < \tilde{\eta} \leq 2^{-d}$, then it follows from properties (ii) and (iv) above as well as Lemma 2.7.20(i) that

$$L_{d,\eta} \setminus \operatorname{Int} L_{d,\tilde{\eta}} = \bigl\{x \in (0,\infty)^d : \tau_{E_d}(x) \in [\eta^{1/d}, \tilde{\eta}^{1/d}]\bigr\} = \textstyle\bigcup_{\lambda \in [1,(\tilde{\eta}/\eta)^{1/d}]} \lambda\, \partial L_{d,\eta}. \tag{2.7.32}$$

In addition, $[0,1/2]^d \cap (\lambda\, \partial L_{d,\eta}) \subseteq \lambda\,([0,1/2]^d \cap \partial L_{d,\eta})$ for all $\lambda > 0$, so by property (vii) and (2.7.31), we can write

$$\begin{aligned}[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}}) &= [0,1/2]^d \cap (L_{d,\eta} \setminus \operatorname{Int} L_{d,\tilde{\eta}}) \\ &= [0,1/2]^d \cap \bigl\{\textstyle\bigcup_{\lambda \in [1,(\tilde{\eta}/\eta)^{1/d}]} \lambda\bigl([0,1/2]^d \cap \partial P_{d,\eta}\bigr)\bigr\} \\ &= [0,1/2]^d \cap \bigl(\textstyle\bigcup_{k=1}^N \bigcup_{\lambda \in [1,(\tilde{\eta}/\eta)^{1/d}]} \lambda R_k\bigr).\end{aligned}$$

By appealing to case (c) of the fact above, we deduce that for every $1 \leq k \leq N$, there is a triangulation of $\bigcup_{\lambda \in [1,(\tilde{\eta}/\eta)^{1/d}]} \lambda R_k$ into d-simplices $T_{k1},\ldots,T_{kd}$, so that

$$[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}}) = \textstyle\bigcup_{k=1}^N \bigcup_{\ell=1}^d \bigl([0,1/2]^d \cap T_{k\ell}\bigr). \tag{2.7.33}$$

Also, for each $1 \leq k \leq N$, recall from the paragraph before (2.7.31) that $R_k \subseteq F_{\eta,m'}$ for some $m' \in \mathbb{Z}^{d-1}$, so by property (iv), it follows that $T_{k\ell} \subseteq \bigcup_{\lambda \in [1,(\tilde{\eta}/\eta)^{1/d}]} \lambda F_{\eta,m'} = \bigcup_{\lambda \in [\eta^{1/d},\, \tilde{\eta}^{1/d}]} \lambda G_{m'}$ for all $1 \leq \ell \leq d$.

Before proceeding, we will now verify that the left hand side of (2.7.33) is in fact the union of those sets $T_{k\ell}^\dagger := [0,1/2]^d \cap T_{k\ell}$ for which $\operatorname{Int} T_{k\ell}^\dagger \neq \emptyset$. In view of (2.7.33) and Lemma 2.7.7, it suffices to show that $[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})$ is the closure of its interior. If $[0,1/2]^d \cap \operatorname{Int} P_{d,\tilde{\eta}} = \emptyset$, then $[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})$ is convex and therefore has the required property by Schneider (2014, Theorem 1.1.15), so suppose now that this is not the case. Fix $\tilde{x} \in \operatorname{Int}([0,1/2]^d \setminus P_{d,\tilde{\eta}})$ and let $x \in [0,1/2]^d \cap (P_{d,\eta} \setminus P_{d,\tilde{\eta}})$. Since $[0,1/2]^d \cap P_{d,\eta}$ is convex, Schneider (2014, Lemma 1.1.9) implies that $[\tilde{x},x) \subseteq \operatorname{Int}([0,1/2]^d \cap P_{d,\eta})$. Also, since $[0,1/2]^d \cap P_{d,\tilde{\eta}}$ is a closed, convex set that does not contain x, there is a unique $x' \in (\tilde{x},x)$ such that $[\tilde{x},x] \cap ([0,1/2]^d \cap P_{d,\tilde{\eta}}) = [\tilde{x},x']$. Therefore,

$$\emptyset \neq (x',x) \subseteq \operatorname{Int}([0,1/2]^d \cap P_{d,\eta}) \cap P_{d,\tilde{\eta}}^c = \operatorname{Int}\{[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})\},$$

so $x \in \operatorname{Cl}(x',x) \subseteq \operatorname{Cl}\operatorname{Int}\{[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})\}$. If instead $x \in [0,1/2]^d \cap \partial P_{d,\tilde{\eta}}$, then $\tau_{E_d}(\lambda x) = \lambda \tau_{E_d}(x) = \lambda \tilde{\eta}^{1/d}$ and $\lambda x \in (0,1/2)^d$ for all $\lambda \in (0,1)$. Thus, if $\lambda \in ((\eta/\tilde{\eta})^{1/d},1)$, then $\lambda x \in \{u \in (0,1/2)^d : \eta^{1/d} < \tau_{E_d}(u) < \tilde{\eta}^{1/d}\} = \operatorname{Int}\{[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})\}$, where the final equality follows from property (iv), (2.7.32) and the continuity of τ_{E_d}. This implies that $x = \lim_{\lambda \nearrow 1} \lambda x \in \operatorname{Cl}\operatorname{Int}\{[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})\}$, as required.

Returning to the proof of (ix), note that for all k,ℓ, the set $T_{k\ell}^\dagger = [0,1/2]^d \cap T_{k\ell}$ is the intersection of a d-simplex and at most $2d$ closed half-spaces, so $T_{k\ell}^\dagger$ is a polytope and the number of vertices of $T_{k\ell}^\dagger$ is bounded above by a constant that depends only on d. Therefore, there exists $\Gamma_d > 0$, depending only on d, such that whenever $\operatorname{Int} T_{k\ell}^{\dagger} \neq \emptyset$, the d-dimensional polytope $T_{k\ell}^{\dagger}$ can be triangulated into at most Γ_d d-simplices (e.g. Rothschild and Straus, 1985, Corollary 2.3), each of which is the convex hull of $d+1$ vertices of $T_{k\ell}^{\dagger}$. It follows from this and the paragraph above that $[0,1/2]^d \cap (P_{d,\eta} \setminus \operatorname{Int} P_{d,\tilde{\eta}})$ can be triangulated into at most $Nd\Gamma_d \leq 2d\Gamma_d\,\alpha'_{d-1}\log^{d-1}(1/\eta)$ d-simplices, in such a way that for each constituent d-simplex T, there exist $1 \leq k \leq N$, $1 \leq \ell \leq d$ and $m' \in \mathbb{Z}^{d-1}$ such that $T \subseteq T_{k\ell} \subseteq \bigcup_{\lambda \in [1,(\tilde{\eta}/\eta)^{1/d}]} \lambda F_{\eta,m'} = \bigcup_{\lambda \in [\eta^{1/d},\,\tilde{\eta}^{1/d}]} \lambda G_{m'}$. This completes the inductive step.

We have now established properties (vi)–(ix), from which we can easily deduce assertions (i) and (ii) of the lemma. To obtain part (iii) of the lemma, recall from Lemma 2.7.19 that $Q^{\triangle}$ is a polytope with $2d$ facets and that $[0,1/(d+1)]^d \subseteq Q^{\triangle} \subseteq [0,1/2]^d$. Thus, $\tilde{P}_\eta = Q^{\triangle} \cap P_\eta$ is a polytope for all $\eta > 0$, and since $[0,1/2]^d \setminus J_\eta \subseteq \frac{d+1}{2}\,([0,1/(d+1)]^d \setminus J_\eta) \subseteq \frac{d+1}{2}\,(Q^{\triangle} \setminus J_\eta)$, it follows from property (vii) above that

$$\begin{aligned}\mu_d(Q^{\triangle} \setminus \tilde{P}_\eta) = \mu_d(Q^{\triangle} \setminus P_\eta) \leq \mu_d([0,1/2]^d \setminus P_\eta) &\leq \alpha'_d\,\mu_d([0,1/2]^d \setminus J_\eta)\\ &\leq \alpha'_d \left(\frac{d+1}{2}\right)^d \mu_d(Q^{\triangle} \setminus J_\eta).\end{aligned}$$

Turning now to part (iv) of the lemma, we first verify that $\tilde{P}_\eta$ is non-empty if and only if $\eta \in (0,(d+1)^{-d}]$. Indeed, if $x = (x_1,\ldots,x_d) \in Q^{\triangle}$, then it follows from the definition of $Q^{\triangle}$ that $1 - \sum_{j=1}^d x_j \leq 1/(d+1)$, so by the AM–GM inequality, we have $\prod_{j=1}^d x_j \leq \bigl(\sum_{j=1}^d x_j/d\bigr)^d \leq (d+1)^{-d}$. Together with the definition of J_η, this implies that $\tilde{P}_\eta = Q^{\triangle} \cap P_\eta \subseteq Q^{\triangle} \cap J_\eta$ is non-empty only if $\eta \in (0,(d+1)^{-d}]$. Conversely, if $\eta \in (0,(d+1)^{-d}]$, then property (iv) above implies that $(\eta^{1/d},\ldots,\eta^{1/d}) \in [0,1/(d+1)]^d \cap P_\eta \subseteq Q^{\triangle} \cap P_\eta = \tilde{P}_\eta$, as required.

For $0 < \eta < \tilde{\eta} \leq (d+1)^{-d}$, we know from property (ix) above that there exist triangulations of $[0,1/2]^d \setminus \operatorname{Int} P_\eta$ and $[0,1/2]^d \cap (P_\eta \setminus \operatorname{Int} P_{d,\tilde{\eta}})$ into at most $\alpha'_d \log(1/\eta)$ d-simplices. Since $Q^{\triangle} \subseteq [0,1/2]^d$, both $Q^{\triangle} \setminus \operatorname{Int} \tilde{P}_{d,\eta} = Q^{\triangle} \cap ([0,1/2]^d \setminus \operatorname{Int} P_\eta)$ and $\tilde{P}_{d,\eta} \setminus \operatorname{Int} \tilde{P}_{d,\tilde{\eta}} = Q^{\triangle} \cap \{[0,1/2]^d \cap (P_\eta \setminus \operatorname{Int} P_{d,\tilde{\eta}})\}$ can be expressed as the union of $Q^{\triangle} \cap T$ over all d-simplices T in the respective triangulations above. By Lemma 2.7.19 and its proof, $Q^{\triangle}$ is the intersection of $2d$ half-spaces, so each set of the form $Q^{\triangle} \cap T$ is the intersection of a d-simplex and $2d$ half-spaces. Arguing as in the proof of (ix) above, we deduce that if $\operatorname{Int}(Q^{\triangle} \cap T) \neq \emptyset$, then $Q^{\triangle} \cap T$ is a d-dimensional polytope that can be triangulated into at most Γ_d simplices, each of which is the convex hull of $d+1$ vertices of $Q^{\triangle} \cap T$.

Moreover, by a very similar argument to that given in the penultimate paragraph of the proof of (ix), the sets $Q^{\triangle} \setminus \operatorname{Int} \tilde{P}_{d,\eta}$ and $\tilde{P}_{d,\eta} \setminus \operatorname{Int} \tilde{P}_{d,\tilde{\eta}}$ are each equal to the closure of their interior. Indeed, note that in common with $[0,1/2]^d$, the set $Q^{\triangle}$ has the property that if $x \in Q^{\triangle}$, then $\lambda x \in \operatorname{Int} Q^{\triangle}$ for all $\lambda \in (0,1)$. Thus, it follows as in the proof of (ix) that $Q^{\triangle} \setminus \operatorname{Int} \tilde{P}_{d,\eta}$ and $\tilde{P}_{d,\eta} \setminus \operatorname{Int} \tilde{P}_{d,\tilde{\eta}}$ can each be expressed as the union of those $Q^{\triangle} \cap T$ for which T is a d-simplex in the corresponding original triangulation and $\operatorname{Int}(Q^{\triangle} \cap T) \neq \emptyset$. We conclude that $Q^{\triangle} \setminus \operatorname{Int} \tilde{P}_{d,\eta}$ and $\tilde{P}_{d,\eta} \setminus \operatorname{Int} \tilde{P}_{d,\tilde{\eta}}$ can each be triangulated into at most $\Gamma_d\,\alpha'_d \log^{d-1}(1/\eta)$ d-simplices, so the proof of part (iv) of the lemma is complete. □

By applying a simple transformation to the polytopes $\tilde{P}_\eta$ from Lemma 2.7.21, we obtain suitable approximating polytopes $P_{\eta,j}^{\triangle}$ for the closed, convex sets $R_j \cap J_\eta^{\triangle} \subseteq \triangle$ defined in Lemma 2.7.19. See Figure 2.1 for an illustration.

Corollary 2.7.22. *There exists $\alpha_d > 0$, depending only on $d \in \mathbb{N}$, such that for every $\eta \in (0,(d+1)^{-d}]$ and every $1 \leq j \leq d+1$, we can construct a polytope $P_{d,\eta,j}^{\triangle} \equiv P_{\eta,j}^{\triangle} \subseteq R_j \cap J_\eta^{\triangle}$ with the following properties:*

(i) $\mu_d(R_j \setminus P_{\eta,j}^{\triangle}) \leq \alpha_d\,\mu_d(R_j \setminus J_\eta^{\triangle})$.

(ii) If $0 < \eta < \tilde{\eta} \leq (d+1)^{-d}$, then $P^{\triangle}_{\tilde{\eta},j} \subsetneq P^{\triangle}_{\eta,j}$, and the regions $R_j \setminus \operatorname{Int} P^{\triangle}_{\eta,j}$ and $P^{\triangle}_{\eta,j} \setminus \operatorname{Int} P^{\triangle}_{\tilde{\eta},j}$ can each be triangulated into at most $\alpha_d \log^{d-1}(1/\eta)$ d-simplices.

Proof. It suffices to establish the result for $j = d+1$, since for any other $1 \leq j \leq d$, there is an (affine) isometry of $\triangle$ that sends $J^{\triangle}_{\eta}$ to itself and maps R_{d+1} to R_j. Writing $\Pi\colon \mathbb{R}^{d+1} \to \mathbb{R}^d$ for the projection onto the first d coordinates, recall from Lemma 2.7.19 that $\tilde{\Pi} := \Pi|_{R_{d+1}} : R_{d+1} \to Q^{\triangle} = \Pi(R_{d+1})$ is a bijection which preserves Lebesgue measure up to a factor of $1/\sqrt{d+1}$. By Lemma 2.7.19(i) and the properties of the sets $P_\eta, \tilde{P}_\eta$ constructed in Lemma 2.7.21, it follows that $P^{\triangle}_{\eta,\,d+1} := \tilde{\Pi}^{-1}(\tilde{P}_\eta) = \tilde{\Pi}^{-1}(Q^{\triangle} \cap P_\eta) \subseteq \tilde{\Pi}^{-1}(Q^{\triangle} \cap J_\eta) = R_{d+1} \cap J^{\triangle}_{\eta}$ for all $\eta \in (0, (d+1)^{-d}]$. Moreover, $P^{\triangle}_{\eta,\,d+1}$ is a polytope since Π is linear and $\tilde{P}_\eta$ is a polytope, and we deduce from Lemma 2.7.21(iii) that

$$\begin{aligned}\mu_d(R_{d+1} \setminus P^{\triangle}_{\eta,\,d+1}) &= \mu_d\bigl(\tilde{\Pi}(R_{d+1} \setminus P^{\triangle}_{\eta,\,d+1})\bigr)/\sqrt{d+1} \\ &= \mu_d(Q^{\triangle} \setminus \tilde{P}_\eta)/\sqrt{d+1} \leq \alpha_d\, \mu_d(Q^{\triangle} \setminus J_\eta)/\sqrt{d+1} = \alpha_d\, \mu_d(R_{d+1} \setminus J^{\triangle}_{\eta}),\end{aligned}$$

where $\alpha_d > 0$ is taken from Lemma 2.7.21 and depends only on d. Finally, if $0 < \eta < \tilde{\eta} \leq (d+1)^{-d}$, then by Lemma 2.7.21(iv), there exist triangulations of $Q^{\triangle} \setminus \operatorname{Int} \tilde{P}_\eta$ and $\tilde{P}_\eta \setminus \operatorname{Int} \tilde{P}_{\tilde{\eta}}$ into at most $\alpha_d \log^{d-1}(1/\eta)$ d-simplices. By applying $\tilde{\Pi}^{-1}$ to all the d-simplices in these triangulations, we obtain suitable triangulations of $R_{d+1} \setminus \operatorname{Int} P^{\triangle}_{\eta,\,d+1} = \tilde{\Pi}^{-1}(Q^{\triangle} \setminus \operatorname{Int} \tilde{P}_\eta)$ and $P^{\triangle}_{\eta,\,d+1} \setminus \operatorname{Int} P^{\triangle}_{\tilde{\eta},\,d+1} = \tilde{\Pi}^{-1}(\tilde{P}_\eta \setminus \operatorname{Int} \tilde{P}_{\tilde{\eta}})$ into at most $\alpha_d \log^{d-1}(1/\eta)$ d-simplices, as required. □

2.8 Supplementary material for Sections 2.4 and 2.5.3

2.8.1 Technical preparation for Section 2.5.3

In this subsection, we restrict attention to the case $d = 3$ and work towards a proof of Proposition 2.5.2 in Section 2.5.3, the key local bracketing entropy bound that implies the main result (Theorem 2.4.3) in Section 2.4. The following two technical lemmas provide pointwise upper and lower bounds on functions f belonging to a δ-Hellinger neighbourhood of some $f_0 \in \mathcal{F}^{(\beta,\Lambda)} \cap \mathcal{F}^{0,I}$. For $g \in \mathcal{F}_d$ and $t \geq 0$, let $U_{g,t} := \{w \in \mathbb{R}^d : g(w) \geq t\}$, which is closed and convex.

Lemma 2.8.1. *Let $d = 3$, and fix $\beta \geq 1$ and $\Lambda > 0$. If $f_0 \in \mathcal{F}^{(\beta,\Lambda)} \cap \mathcal{F}^{0,I}$ and $f \in \tilde{\mathcal{F}}(f_0, \delta)$ for some $\delta > 0$, then $f(x) \geq f_0(x)/2$ for all $x \in \mathbb{R}^3$ satisfying $f_0(x) \geq (\tilde{c}\Lambda^3\delta^2)^{\beta/(\beta+3)}$, where $\tilde{c} := 6144\pi^{-1}$.*

Proof. Fix $x \in \mathbb{R}^3$ with $f_0(x) \geq (\tilde{c}\Lambda^3\delta^2)^{\beta/(\beta+3)}$. It can be assumed without loss of generality that $f(x) < f_0(x)$, and we begin by setting

$$t := \frac{f_0(x) - f(x)}{2}, \quad U := U_{f,\,f(x)}, \quad U_H := U_{f_0,\,f_0(x)} \quad \text{and} \quad U_L := U_{f_0,\,f_0(x)-t}.$$

Then it follows from the defining condition (2.4.1) for $\mathcal{F}^{(\beta,\Lambda)}$ that

$$\min_{y \in \partial U_L} \min_{z \in \partial U_H} \|y - z\| \geq \frac{t\Lambda^{-1}}{f_0(x)^{1-1/\beta}} =: \tilde{r}. \tag{2.8.1}$$

Also, note that there exists $u \in \mathbb{R}^3 \setminus \{0\}$ such that $f \leq f(x)$ on $H^+_{x,u} := \{w \in \mathbb{R}^3 : u^\top w \geq u^\top x\}$. Indeed, this is clear if $f(x) = \max_{w \in \mathbb{R}^3} f(w)$, and in the case where $f(x) < \max_{w \in \mathbb{R}^3} f(w)$, we have $x \in \partial U$ by the concavity of $\log f$, so there exists a suitable supporting half-space to U at x.

Next, we fix $x' \in \operatorname{argmax}_{w \in U_H} u^\top w$ (which necessarily lies in ∂U_H) and apply (2.8.1) to deduce that $\bar{B}(x', \tilde{r}) \cap H^+_{x',u} \subseteq (U_L \setminus \operatorname{Int} U_H) \cap H^+_{x,u}$, where $H^+_{x',u} := \{w \in \mathbb{R}^3 : u^\top w \geq u^\top x'\}$. Since

$f_0 \geq f_0(x) - t$ on $(U_L \setminus \operatorname{Int} U_H)$ and $f \leq f(x) = f_0(x) - 2t$ on $H^+_{x,u}$, we have

$$\delta^2 \geq \int_{(U_L \setminus \operatorname{Int} U_H)\cap H^+_{x,u}} \bigl(f_0^{1/2} - f^{1/2}\bigr)^2 \geq \bigl(\sqrt{f_0(x)-t} - \sqrt{f_0(x)-2t}\bigr)^2 \mu_3\bigl(\bar{B}(x',\tilde{r}) \cap H^+_{x',u}\bigr)$$
$$= \frac{2\pi}{3}\bigl(\sqrt{f_0(x)-t} - \sqrt{f_0(x)-2t}\bigr)^2 \biggl(\frac{t\Lambda^{-1}}{f_0(x)^{1-1/\beta}}\biggr)^3. \quad (2.8.2)$$

Now since

$$\sqrt{f_0(x)-t} - \sqrt{f_0(x)-2t} = \frac{t}{\sqrt{f_0(x)-t} + \sqrt{f_0(x)-2t}} \geq \frac{t}{2\sqrt{f_0(x)}},$$

it follows from (2.8.2) that

$$\delta^2 \geq \frac{\pi\, t^5 \Lambda^{-3}}{6 f_0(x)^{4-3/\beta}},$$

so $\{f_0(x) - f(x)\}/2 = t \leq (6/\pi)^{1/5}\, \delta^{2/5}\, \Lambda^{3/5}\, f_0(x)^{\frac{4}{5}-\frac{3}{5\beta}}$. Rearranging this, we obtain the bound

$$f(x) \geq f_0(x) - 2(6/\pi)^{1/5}\, \delta^{2/5}\, \Lambda^{3/5}\, f_0(x)^{\frac{4}{5}-\frac{3}{5\beta}}. \quad (2.8.3)$$

The right hand side of (2.8.3) is bounded below by $f_0(x)/2$ if and only if

$$f_0(x) \geq (6 \times 4^5/\pi)^{\beta/(\beta+3)}\, \Lambda^{3\beta/(\beta+3)}\, \delta^{2\beta/(\beta+3)} = (\tilde{c}\Lambda^3\delta^2)^{\beta/(\beta+3)}.$$

This completes the proof. □

Lemma 2.8.2. *Let $d = 3$, and fix $\beta \geq 1$ and $\Lambda > 0$. There exists a universal constant $\tilde{c}' > 0$ such that whenever $0 < \delta < e^{-1} \wedge (\tilde{c}'\Lambda^{-3/2}\log_+^{-1}\Lambda)$, $f_0 \in \mathcal{F}^{(\beta,\Lambda)} \cap \mathcal{F}^{0,I}$ and $f \in \tilde{\mathcal{F}}(f_0,\delta) \cap \tilde{\mathcal{F}}^{1,\eta}$, we have $f(x) \lesssim f_0(x) \vee \{\Lambda^3\delta^2\log^2(\Lambda^{-3}\delta^{-2})\}^{\beta/(\beta+3)}$ for all $x \in \mathbb{R}^3$.*

Proof. Since the bound (2.5.33) applies to $f \in \tilde{\mathcal{F}}^{1,\eta}$, there exists a universal constant $\tilde{C}_3 > 0$ such that $f(x) \leq \Lambda^3\delta^2$ whenever $\|x\| > \tilde{C}_3 \log(\Lambda^{-3}\delta^{-2})$. Moreover, if $f_0(x) \geq 2^{-8d}/6 = 2^{-24}/6 =: c_0$, then it follows from (2.5.33) that

$$f(x) \leq \exp(\tilde{b}_3) \leq c_0^{-1}\exp(\tilde{b}_3) f_0(x).$$

Thus, we may restrict attention to $x \in \mathbb{R}^3$ such that $\|x\| \leq \tilde{C}_3\log(\Lambda^{-3}\delta^{-2})$, $f_0(x) < c_0$ and $f(x) > f_0(x)$. Fixing such an x, we will show that there exist universal constants $C'' > C' > 0$ with

$$f(x) \leq 3f_0(x) \quad \text{if } f_0(x) \geq C't; \quad (2.8.4)$$
$$f(x) \leq 2C''t \quad \text{otherwise}, \quad (2.8.5)$$

where $t := \{\Lambda^3\delta^2\log^2(\Lambda^{-3}\delta^{-2})\}^{\beta/(\beta+3)}$. First, since $f_0 \in \mathcal{F}^{0,I}$, it follows from Lovász and Vempala (2006, Theorem 5.14) that $\inf_{\|w\|\leq 1/9} f_0(w) \geq 2^{-8d} = 6c_0$, and hence that $\|x\| > 1/9$. Also, Lemma 2.8.1 implies that $\inf_{\|w\|\leq 1/9} f(w) \geq \inf_{\|w\|\leq 1/9} f_0(w)/2 \geq 3c_0$, provided that

$$6c_0 \geq (\tilde{c}\Lambda^3\delta^2)^{\beta/(\beta+3)}. \quad (2.8.6)$$

In addition, let $s := \bigl(f_0(x) + \{f(x) \wedge (3c_0)\}\bigr)/2$ and $H_x := \{w \in \mathbb{R}^d : w^\top x = 0\}$. Since f is log-concave, we have $f(w) \geq f(x) \wedge (3c_0) = 2s - f_0(x)$ for all $w \in \operatorname{conv}\bigl(\{\bar{B}(0,1/9) \cap H_x\} \cup \{x\}\bigr) =: K$. Note that K is a cone of volume $\mu_3(K) = 9^{-2}\,\pi\|x\|/3$.

Since $f_0 \in \mathcal{F}^{(\beta,\Lambda)}$ and $f_0(x) < s$, we have $f_0(w) < s$ for all $w \in \bar{B}(x,r')$, where $r' := \Lambda^{-1}\{s - f_0(x)\}/s^{1-1/\beta}$. Therefore, $f(w) \geq 2s - f_0(x) > s > f_0(w)$ for all $w \in K \cap \bar{B}(x,r') =: K'$. Noting that $K' - x \supseteq \bigl(r'/\sqrt{\|x\|^2 + 9^{-2}}\bigr)(K - x)$ and recalling that $\|x\| > 1/9$, we deduce that

$$\mu_3(K') \geq \left(\frac{r'}{\sqrt{\|x\|^2 + 9^{-2}}}\right)^3 \mu_3(K) \gtrsim \left(\frac{s - f_0(x)}{\Lambda s^{1-1/\beta}}\right)^3 \|x\|^{-2}.$$

Now since $\|x\| \leq \tilde{C}_3 \log(\Lambda^{-3}\delta^{-2})$, it follows that

$$\delta^2 \geq \int_{K'} \bigl(f^{1/2} - f_0^{1/2}\bigr)^2 \gtrsim \bigl(\sqrt{2s - f_0(x)} - \sqrt{s}\bigr)^2 \left(\frac{s - f_0(x)}{\Lambda s^{1-1/\beta}}\right)^3 \log^{-2}(\Lambda^{-3}\delta^{-2}),$$

which implies that

$$t^{(\beta+3)/\beta} = \Lambda^3\, \delta^2 \log^2(\Lambda^{-3}\delta^{-2}) \gtrsim \frac{\{s - f_0(x)\}^5}{s^{3\,(1-1/\beta)}\bigl(\sqrt{2s - f_0(x)} + \sqrt{s}\bigr)^2} \gtrsim \frac{\{s - f_0(x)\}^5}{s^{4-3/\beta}}.$$

This shows that

$$s^\alpha - f_0(x)s^{\alpha-1} \leq Ct^\alpha, \tag{2.8.7}$$

where $\alpha := (\beta + 3)/(5\beta) \in (0, 1)$ and $C > 0$ is a suitable universal constant. For our fixed $x \in \mathbb{R}^3$, we see that the function $g\colon [f_0(x), \infty) \to [0, \infty)$ defined by $g(w) := w^\alpha - f_0(x)w^{\alpha-1}$ is strictly increasing. Observe also that there exists a universal constant $C' > 0$ such that if $f_0(x) \geq C't$, then $g(2f_0(x)) \geq Ct^\alpha \geq g(s)$. In this case, it follows from (2.8.7) that

$$\bigl(f_0(x) + \{f(x) \wedge (3c_0)\}\bigr)/2 = s \leq 2f_0(x)$$

and hence that $f(x) \wedge (3c_0) \leq 3f_0(x)$. But since it was assumed that $f_0(x) < c_0$, we deduce that $f(x) \leq 3f_0(x)$, which yields (2.8.4).

Otherwise, if $f_0(x) < C't$, then $g(w) \geq w^\alpha - C'tw^{\alpha-1}$ for $w \geq f_0(x)$, so there exists a universal constant $C'' > C'$ such that $g(C''t) \geq Ct^\alpha \geq g(s)$. As above, we deduce from (2.8.7) that $s \leq C''t$, and so long as

$$3c_0 > 2C''t, \tag{2.8.8}$$

this yields the desired bound (2.8.5). It is easy to verify that there exists a universal constant $\tilde{c}' > 0$ such that (2.8.6) and (2.8.8) are satisfied whenever $0 < \delta < e^{-1} \wedge (\tilde{c}'\Lambda^{-3/2} \log_+^{-1} \Lambda)$. This completes the proof. □

In the proof of Proposition 2.5.2, we also apply the following geometric result, which is due to Bronshteyn and Ivanov (1975).

Lemma 2.8.3. *For each $d \in \mathbb{N}$, there exist $\bar{\eta} \equiv \bar{\eta}_d > 0$ and $\bar{C}^* \equiv \bar{C}^*_d > 0$, depending only on d, such that for each $\eta \in (0, \bar{\eta})$ and each compact, convex $D \subseteq \bar{B}(0, 1) \subseteq \mathbb{R}^d$, we can find a polytope P with at most $\bar{C}^*\eta^{-(d-1)/2}$ vertices with the property that $D \subseteq P \subseteq D + \bar{B}(0, \eta)$.*

2.8.2 Hölder classes

First, we extend the notions of Hölder regularity discussed in Section 2.4 in the main text to general exponents $\beta > 1$. It will be helpful to introduce the following additional notation. For finite-dimensional vector spaces V, W over $\mathbb{R}$, let $\mathcal{L}(V, W) \equiv \mathcal{L}^{(1)}(V, W)$ denote the $\{\dim(V) \times \dim(W)\}$-dimensional vector space of all linear maps from V to W. For positive integers $k \geq 2$, we inductively define $\mathcal{L}^{(k)}(V, W) := \mathcal{L}\bigl(V, \mathcal{L}^{(k-1)}(V, W)\bigr)$. This may be identified with the space of all k-linear maps from $V^k = V \times \cdots \times V$ to W, or equivalently the space $\mathcal{L}(V^{\otimes k}, W)$, where $V^{\otimes k} = V \otimes \cdots \otimes V$ denotes the k-fold tensor product of V with itself. For $k \in \mathbb{N}$ and a linear map $T\colon V \to W$, we write

$T^{\otimes k}\colon V^{\otimes k} \to W^{\otimes k}$ for the k-fold tensor product of T with itself, which sends $u_1 \otimes \cdots \otimes u_k \in V^{\otimes k}$ to $Tu_1 \otimes \cdots \otimes Tu_k \in W^{\otimes k}$. When $V = \mathbb{R}^d$ for some $d \in \mathbb{N}$ and $W = \mathbb{R}$, we define the Hilbert–Schmidt norm on $\mathcal{L}\big((\mathbb{R}^d)^{\otimes k}, \mathbb{R}\big)$ for $k \in \mathbb{N}$ by

$$\|\alpha\|_{\mathrm{HS}} := \mathrm{tr}(\alpha\alpha^*)^{\frac{1}{2}} = \mathrm{tr}(\alpha^*\alpha)^{\frac{1}{2}} = \Bigg(\sum_{i_1,\ldots,i_k=1}^{d} \alpha(e_{i_1} \otimes \cdots \otimes e_{i_k})^2\Bigg)^{\frac{1}{2}}, \tag{2.8.9}$$

where $\alpha^* \in \mathcal{L}\big(\mathbb{R}, (\mathbb{R}^d)^{\otimes k}\big)$ denotes the adjoint of α (as a linear map between inner product spaces). In an abuse of notation, we also write $\|\cdot\|_{\mathrm{HS}}$ for the norm this induces on $\mathcal{L}^{(k)}(\mathbb{R}^d, \mathbb{R})$. This is the natural analogue of the Frobenius norm for general multilinear forms; indeed, when $k = 2$, the expression in (2.8.9) coincides with the Frobenius norm of the matrix that represents the symmetric bilinear form corresponding to α with respect to the standard basis of $\mathbb{R}^d$.

The reason for making these definitions is that if $f\colon V \to W$ is a map between finite-dimensional normed spaces and f is differentiable at $x \in V$, then the derivative of f at x, written $Df(x)$, is an element of $\mathcal{L}(V, W)$. In particular, if f is itself linear, then $Df(x) = f$ for all $x \in V$. More generally, if $k \in \mathbb{N}$ and $f\colon V \to W$ is $(k-1)$ times differentiable in a neighbourhood of $x \in V$ and k times differentiable at x, then the kth derivative of f at x, written $D^k f(x)$, is an element of $\mathcal{L}^{(k)}(V, W)$. It is conventional to regard $D^k f(x)$ as a k-linear map $(u_1, \ldots, u_k) \mapsto D^k f(x)(u_1, \ldots, u_k)$. By repeatedly applying the chain rule, we can establish the following:

Lemma 2.8.4. *Let $f\colon \mathbb{R}^d \to \mathbb{R}$ be k times differentiable for some $k \in \mathbb{N}$ and let $T\colon \mathbb{R}^m \to \mathbb{R}^d$ be a linear map. Then $D^k(f \circ T)(x)(u_1, \ldots, u_k) = D^k f(Tx)(Tu_1, \ldots, Tu_k)$ for all $x, u_1, \ldots, u_k \in \mathbb{R}^m$. Equivalently, if we view $D^k(f \circ T)(x)$ and $D^k f(x)$ as elements of $\mathcal{L}\big((\mathbb{R}^m)^{\otimes k}, \mathbb{R}\big)$ and $\mathcal{L}\big((\mathbb{R}^d)^{\otimes k}, \mathbb{R}\big)$ respectively, then $D^k(f \circ T)(x) = D^k f(x) \circ T^{\otimes k}$.*

Proof. For $k \in \mathbb{N}$, let us define the dual map $(T^{\otimes k})^*\colon \mathcal{L}\big((\mathbb{R}^d)^{\otimes k}, \mathbb{R}\big) \to \mathcal{L}\big((\mathbb{R}^m)^{\otimes k}, \mathbb{R}\big)$ to $T^{\otimes k}$ by $(T^{\otimes k})^*(\alpha) := \alpha \circ T^{\otimes k}$, and write $T_{(k)}$ for the corresponding linear map from $\mathcal{L}^{(k)}(\mathbb{R}^d, \mathbb{R})$ to $\mathcal{L}^{(k)}(\mathbb{R}^m, \mathbb{R})$. Viewing $D^k(f \circ T)(x)$ and $D^k f(x)$ as elements of $\mathcal{L}^{(k)}(\mathbb{R}^m, \mathbb{R})$ and $\mathcal{L}^{(k)}(\mathbb{R}^d, \mathbb{R})$ respectively, we will establish by induction on k that $D^k(f \circ T)(x) = T_{(k)} \circ D^k f(Tx)$ for all $k \in \mathbb{N}$, which implies the desired conclusion. The base case $k = 1$ follows by applying the chain rule directly to the function $f \circ T$. For a general $k \geq 2$, the inductive hypothesis asserts that $D^{k-1}(f \circ T)(x) = (T_{(k-1)} \circ g_{k-1})(x)$, where $g_{k-1}(x) := D^{k-1} f(Tx)$, and we deduce by a further application of the chain rule that $Dg_{k-1}(x) = D^k(Tx) \circ T$. Recalling that $T_{(k-1)}$ is linear, we apply the chain rule once again to conclude that

$$\begin{aligned} D^k(f \circ T)(x) = D(T_{(k-1)} \circ g_{k-1})(x) &= T_{(k-1)} \circ Dg_{k-1}(x) \\ &= T_{(k-1)} \circ D^k f(Tx) \circ T = T_{(k)} \circ D^k f(Tx), \end{aligned}$$

as required. □

Using the above notation, we are now ready to formulate definitions of β-Hölder regularity for functions defined on $\mathbb{R}^d$ for general $\beta > 1$ and $d \in \mathbb{N}$. For $\beta > 1$ and $L > 0$, we say that $h\colon \mathbb{R}^d \to \mathbb{R}$ is (β, L)-*Hölder* on $\mathbb{R}^d$ if h is $k := \lceil \beta \rceil - 1$ times differentiable on $\mathbb{R}^d$ and

$$\|D^k h(y) - D^k h(x)\|_{\mathrm{HS}} \leq L\|y - x\|^{\beta - k} \tag{2.8.10}$$

for all $x, y \in \mathbb{R}^d$. We say that h is β-*Hölder* if there exists $L > 0$ such that h is (β, L)-Hölder. It is convenient to let $\mathsf{H}(\beta, L) \equiv \mathsf{H}_d(\beta, L)$ denote the class of (β, L)-*Hölder* densities on $\mathbb{R}^d$.

In addition, we seek to extend the definition (2.4.6) of the affine invariant classes $\mathcal{H}^{\beta,L}$ in Example 2.5 (in Section 2.4 in the main text) to encompass general $\beta > 1$, rather than confine ourselves to working with $\beta \in (1,2]$. To this end, we define a scaled version of (2.8.9) for each $S \in \mathbb{S}^{d\times d}$ by

$$\|\alpha\|_S' := \Bigl\|\alpha \circ (S^{-1/2})^{\otimes k}\Bigr\|_{\mathrm{HS}} \det{}^{-1/2} S = \left\{\sum_{i_1,\dots,i_k=1}^{d} \alpha\bigl(S^{-1/2}e_{i_1} \otimes \cdots \otimes S^{-1/2}e_{i_k}\bigr)^2 \det{}^{-1} S\right\}^{1/2}; \tag{2.8.11}$$

since $(S^{-1/2})^{\otimes k}$ is invertible with inverse $(S^{1/2})^{\otimes k}$, we see that $\|\cdot\|_S'$ does indeed constitute a norm on $\mathcal{L}\bigl((\mathbb{R}^d)^{\otimes k}, \mathbb{R}\bigr)$. In a further abuse of notation, we also write $\|\cdot\|_S'$ for the corresponding norm on $\mathcal{L}^{(k)}(\mathbb{R}^d, \mathbb{R})$. Now for general $\beta > 1$ and $L > 0$, denote by $\mathsf{H}_*(\beta, L)$ the collection of all densities f on $\mathbb{R}^d$ for which f is $k := \lceil \beta \rceil - 1$ times differentiable on $\mathbb{R}^d$ and

$$\|D^k f(y) - D^k f(x)\|_{\Sigma_f^{-1}}' \leq L\|y - x\|_{\Sigma_f}^{\beta - k} \tag{2.8.12}$$

for all $x, y \in \mathbb{R}^d$, where the norm on the left-hand side is given by (2.8.11). Note that when $\beta \in (1,2]$ or $\beta \in (2,3]$, our previous definitions (2.4.6) and (2.4.7) of the classes $\mathcal{H}^{\beta,L}$ in the main text satisfy $\mathcal{H}^{\beta,L} = \mathsf{H}_*(\beta, L) \cap \mathcal{F}_d$. We now verify that:

Lemma 2.8.5. *For general $\beta > 1$ and $L > 0$, the class $\mathsf{H}_*(\beta, L)$ is affine invariant.*

Proof. Fix $f \in \mathsf{H}_*(\beta, L)$ and define a density g on $\mathbb{R}^d$ by

$$g(x) := \frac{1}{|\det A|} f\bigl(A^{-1}(x - b)\bigr),$$

where $b \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d\times d}$ is invertible. Since $\Sigma_g = A\Sigma_f A^\top$, every $\alpha \in \mathcal{L}\bigl((\mathbb{R}^d)^{\otimes k}, \mathbb{R}\bigr)$ satisfies

$$\begin{aligned}\Bigl\|\alpha \circ (A^{-1}\Sigma_g^{1/2})^{\otimes k}\Bigr\|_{\mathrm{HS}} &= \mathrm{tr}\Bigl(\alpha \circ \bigl\{A^{-1}\Sigma_g(A^{-1})^\top\bigr\}^{\otimes k} \circ \alpha^*\Bigr)^{1/2} \\ &= \mathrm{tr}\bigl(\alpha \circ \Sigma_f^{\otimes k} \circ \alpha^*\bigr)^{1/2} = \bigl\|\alpha \circ (\Sigma_f^{1/2})^{\otimes k}\bigr\|_{\mathrm{HS}}.\end{aligned} \tag{2.8.13}$$

Setting $k := \lceil \beta \rceil - 1$ and viewing $D^k f(x)$ and $D^k g(x)$ as elements of the space $\mathcal{L}\bigl((\mathbb{R}^d)^{\otimes k}, \mathbb{R}\bigr)$, we deduce from Lemma 2.8.4 and (2.8.13) that

$$\begin{aligned}&\|D^k g(y) - D^k g(x)\|_{\Sigma_g^{-1}}' \\ &\quad= \bigl\|\bigl\{D^k f\bigl(A^{-1}(y-b)\bigr) - D^k f\bigl(A^{-1}(x-b)\bigr)\bigr\} \circ (A^{-1})^{\otimes k}\bigr\|_{\Sigma_g^{-1}} \\ &\quad= \Bigl\|\bigl\{D^k f\bigl(A^{-1}(y-b)\bigr) - D^k f\bigl(A^{-1}(x-b)\bigr)\bigr\} \circ (A^{-1}\Sigma_g^{1/2})^{\otimes k}\Bigr\|_{\mathrm{HS}} \det{}^{1/2}\Sigma_f \\ &\quad= \bigl\|\bigl\{D^k f\bigl(A^{-1}(y-b)\bigr) - D^k f\bigl(A^{-1}(x-b)\bigr)\bigr\} \circ (\Sigma_f^{1/2})^{\otimes k}\bigr\|_{\mathrm{HS}} \det{}^{1/2}\Sigma_f \\ &\quad= \bigl\|D^k f\bigl(A^{-1}(y-b)\bigr) - D^k f\bigl(A^{-1}(x-b)\bigr)\bigr\|_{\Sigma_f^{-1}} \\ &\quad\leq L\|A^{-1}(y-x)\|_{\Sigma_f}^{\beta-k} = L\|y-x\|_{\Sigma_g}^{\beta-k}\end{aligned}$$

for all $x, y \in \mathbb{R}^d$, as required. □

Next, we establish that for all $\beta > 1$, the classes $\mathsf{H}(\beta, L)$ of (β, L)-Hölder densities on $\mathbb{R}^d$ are nested with respect to the Hölder exponent β in the sense of part (ii) of the result below.

Proposition 2.8.6. *For each $d \in \mathbb{N}$, we have the following:*

(i) For $\beta > 1$ and $L > 0$, there exists $C \equiv C(d,\beta,L) > 0$ such that, writing $k := \lceil \beta \rceil - 1$, we have

$$\max_{j=0,1,\ldots,k} \sup_{f \in \mathsf{H}(\beta,L)} \sup_{x \in \mathbb{R}^d} \|D^j f(x)\|_{\mathrm{HS}} \leq C.$$

(ii) For $\beta > 1$ and $L > 0$, there exists $\tilde{L} \equiv \tilde{L}(d,\beta,L) > 0$ such that $\mathsf{H}(\beta,L) \subseteq \mathsf{H}(\alpha,\tilde{L})$ and $\mathsf{H}_*(\beta,L) \subseteq \mathsf{H}_*(\alpha,\tilde{L})$ for all $\alpha \in (1,\beta]$.

Proof. (i) Let φ denote the standard normal density on $\mathbb{R}$ and, for $r \in \mathbb{N}_0$, let H_r denote the rth Hermite polynomial, given by $H_r(u) := (-1)^r \varphi^{(r)}(u)/\varphi(u)$. Now define $K \colon \mathbb{R} \to \mathbb{R}$ by

$$K(u) := \sum_{r=0}^{k} \frac{H_r(0)H_r(u)}{(2\pi)^{1/2} r!} e^{-u^2/2},$$

so that K is bounded, infinitely differentiable and satisfies $\int_{-\infty}^{\infty} K(u)\,du = 1$, $\int_{-\infty}^{\infty} u^j K(u)\,du = 0$ for $j = 1,\ldots,k$ and $K^{(j)}(u) \to 0$ as $u \to \pm\infty$ for $j \in \mathbb{N}_0$ (Tsybakov, 2009, pp. 10–12). Now, for $u \equiv (u_1,\ldots,u_d) \in \mathbb{R}^d$, define the product kernel K_d by $K_d(u) := \prod_{j=1}^d K(u_j)$, and note that for every $\alpha > 0$, we have $\mu_\alpha(K_d) := \int_{\mathbb{R}^d} \|u\|^\alpha |K_d(u)|\,du < \infty$.

Fix $j \in \{0,1,\ldots,k\}$, let $\mathcal{J}_j := \bigl\{\mathbf{j} \equiv (j_1,\ldots,j_d) \in \mathbb{N}_0^d : j_1 + \ldots + j_d = j\bigr\}$ and note that $\mathcal{J}_j = \binom{k-j+d-1}{d-1}$. With standard multi-index notation for partial derivatives, for $\mathbf{j} \in \mathcal{J}_j$ and some $\tau_{\mathbf{j}} \in [0,1]$, we can write

$$\begin{aligned}
\biggl|\int_{\mathbb{R}^d} K_d(x-z) D_{\mathbf{j}} f(z)\,dz - D_{\mathbf{j}} f(x)\biggr| &= \biggl|\int_{\mathbb{R}^d} K_d(u)\bigl\{D_{\mathbf{j}} f(x-u) - D_{\mathbf{j}} f(x)\bigr\}\,du\biggr| \\
&\leq \biggl|\int_{\mathbb{R}^d} K_d(u)\biggl[\sum_{\ell=j+1}^{k-1} \sum_{\mathbf{r} \in \mathcal{J}_{\ell-j}} \prod_{s=1}^d \frac{(-u_s)^{r_s}}{r_s!} D_{\mathbf{j}+\mathbf{r}} f(x) \\
&\quad + \sum_{\mathbf{r} \in \mathcal{J}_{k-j}} \prod_{s=1}^d \frac{(-u_s)^{r_s}}{r_s!}\bigl\{D_{\mathbf{j}+\mathbf{r}} f(x-\tau_{\mathbf{j}} u) - D_{\mathbf{j}+\mathbf{r}} f(x)\bigr\}\biggr]\,du\biggr| \\
&\leq L^d \sum_{\mathbf{r} \in \mathcal{J}_{k-j}} \int_{\mathbb{R}^d} \prod_{s=1}^d |u_s|^{r_s} \|u\|^{\beta-k} |K_d(u)|\,du \\
&\leq L^d \binom{k-j+d-1}{d-1} \mu_{\beta-j}(K_d).
\end{aligned} \tag{2.8.14}$$

In particular, with $j = 0$, we have

$$\begin{aligned}
f(x) &\leq \int_{\mathbb{R}^d} |K_d(x-z)|\, f(z)\,dz + \biggl|\int_{\mathbb{R}^d} K_d(x-z) f(z)\,dz - f(x)\biggr| \\
&\leq \|K_d\|_\infty + L^d \binom{k+d-1}{d-1} \mu_\beta(K_d).
\end{aligned}$$

Now fix $j \in \mathbb{N}$ and suppose as an inductive hypothesis that

$$\sup_{f \in \mathsf{H}(\beta,L)} \sup_{x \in \mathbb{R}^d} \|D^\ell f(x)\|_{\mathrm{HS}} \leq C$$

for $\ell = 1,\ldots,j-1$. Then, for $\mathbf{j} = (j_1,\ldots,j_d) \in \mathcal{J}_j$, applying Fubini's theorem and integrating by parts one coordinate at a time, we obtain

$$\int_{\mathbb{R}^d} K_d(x-z) D_{\mathbf{j}} f(z)\,dz = (-1)^j \int_{\mathbb{R}^d} D_{\mathbf{j}} K_d(x-z) f(z)\,dz, \tag{2.8.15}$$

where we have used the inductive hypothesis to argue that the integrated terms vanish, since $|D_{\mathbf{j}'}K_d(x-z)||D_{\mathbf{j}''-\mathbf{j}'}f(z)| \leq C|D_{\mathbf{j}'}K_d(x-z)| \to 0$ as $\|z\| \to \infty$ whenever $\mathbf{j}' = (j_1', \ldots, j_d') \in \mathcal{J}_{j-1}$ and $\mathbf{j}'' = (j_1'', \ldots, j_d'') \in \mathcal{J}_{j-1}$ satisfy $j_s' \leq j_s'' \leq j_s$ for all $s = 1, \ldots, d$. It follows from (2.8.14) and (2.8.15) that for all $f \in \mathsf{H}(\beta, L)$ and $x \in \mathbb{R}^d$,

$$\begin{aligned}\|D^j f(x)\|_{\mathrm{HS}} &\leq d^{j/2} \max_{\mathbf{j}\in\mathcal{J}_j} \biggl\{ \biggl| \int_{\mathbb{R}^d} K_d(x-z) D_{\mathbf{j}} f(z)\,dz \biggr| + \biggl| \int_{\mathbb{R}^d} K_d(x-z) D_{\mathbf{j}} f(z)\,dz - D_{\mathbf{j}} f(x) \biggr| \biggr\} \\ &\leq d^{j/2} \biggl\{ \max_{\mathbf{j}\in\mathcal{J}_j} \sup_{u\in\mathbb{R}^d} |D_{\mathbf{j}} K(u)| + L^d \binom{k-j+d-1}{d-1} \mu_{\beta-j}(K_d) \biggr\},\end{aligned}$$

which proves the desired result by induction.

(ii) Fix $\beta > 1$ and $L > 0$ and consider any $f \in \mathsf{H}(\beta, L)$. Let $\tilde{L} := L \vee (2C)$ and note that if $\alpha \in (1, \beta]$, then writing $k := \lceil \beta \rceil - 1$ we have that

$$\|D^k f(y) - D^k f(x)\|_{\mathrm{HS}} \leq L\|y-x\|^{\beta-k} \leq L\|y-x\|^{\alpha-k} \leq \tilde{L}\|y-x\|^{\alpha-k}$$

whenever $\|y-x\| \leq 1$. On the other hand, if $\|y-x\| > 1$, then

$$\|D^k f(y) - D^k f(x)\|_{\mathrm{HS}} \leq 2C < \tilde{L}\|y-x\|^{\alpha-k}.$$

This proves that $\mathsf{H}(\beta, L) \subseteq \mathsf{H}(\alpha, \tilde{L})$. For the final claim, it suffices by the affine invariance of $\mathsf{H}_*(\beta, L)$ (Lemma 2.8.5) to prove the result for isotropic densities; but this is precisely what we proved in the first part of (ii). □

Remark. For $\beta > 1$, this argument shows that classes of β-Hölder *densities* defined on the whole of $\mathbb{R}^d$ are nested with respect to β. However, the same is not true of classes of general β-Hölder functions on $\mathbb{R}^d$; see the discussion at the end of Example 2.4 in Section 2.4 in the main text.

Proposition 2.8.7 shows that the classes $\tilde{\mathcal{H}}^{\gamma,L}$ and $\mathcal{H}^{\beta,L}$ defined in Examples 2.4 and 2.5 respectively (in Section 2.4 in the main text) are contained within the more general classes $\mathcal{F}^{(\beta',\Lambda')}$ for suitably chosen values of β' and Λ' in each case.

Proposition 2.8.7. *For $L > 0$, we have the following:*

(i) If $\beta \in (1,2]$, then every $f \in \mathcal{H}^{\beta,L}$ satisfies (2.4.2) and therefore (2.4.1) with this value of β and $\Lambda = \Lambda(\beta, L) := L^{1/\beta}(1-1/\beta)^{-1+1/\beta}$. Consequently, $\mathcal{H}^{\beta,L} \subseteq \mathcal{F}^{(\beta,\,\Lambda(\beta,L))}$.

(ii) For $\beta \in (1,2]$, suppose that $g\colon \mathbb{R}^d \to [0,\infty)$ satisfies $\|\nabla g(y) - \nabla g(x)\| \leq L\|y-x\|^{\beta-1}$ for all $x, y \in \mathbb{R}^d$. Then $\|\nabla g(x)\| \leq \Lambda(\beta, L)\, g(x)^{1-1/\beta}$ for all $x \in \mathbb{R}^d$ and $\|x-y\| \geq \Lambda^{-1}(\beta, L)\{g(x) - g(y)\}/g(x)^{1-1/\beta}$ whenever $x, y \in \mathbb{R}^d$ satisfy $g(x) > g(y)$.

(iii) If $\beta \in (2,3]$, then there exists $\Lambda \equiv \Lambda(\beta, L) > 0$ such that every $f \in \mathcal{H}^{\beta,L}$ satisfies (2.4.2) and therefore (2.4.1) with this value of β and $\Lambda = \Lambda(\beta, L)$. Consequently, $\mathcal{H}^{\beta,L} \subseteq \mathcal{F}^{(\beta,\,\Lambda(\beta,L))}$.

(iv) If $\beta' \geq 1$ and $\gamma \in (1,2]$, then there exists $\bar{B} \equiv \bar{B}_d > 0$ depending only on d such that every $f \in \tilde{\mathcal{H}}^{\gamma,L}$ satisfies (2.4.2) and therefore (2.4.1) with $\beta = \beta'$, $\Lambda = \beta\Lambda(\gamma, L)\bar{B}$ and any $\tau \leq e^{-1}$. Consequently, for any $\beta \geq 1$, we have $\bigcup_{\gamma\in[1,2]} \tilde{\mathcal{H}}^{\gamma,L} \subseteq \mathcal{F}^{(\beta,\,\Lambda'(\beta,L))}$, where $\Lambda'(\beta, L) := \beta(L \vee L^{1/2})\bar{B}e^{1/e}(eB_d)^{1/\beta}$ and $B_d > 0$ is taken from Proposition 2.4.1(ii).

Proof. As in the proof of Proposition 2.4.2, we write $\Sigma \equiv \Sigma_f$ for convenience and let $\langle v, w\rangle' := (\det\Sigma)\,(v^\top\Sigma w)$ denote the inner product that gives rise to the norm $\|\cdot\|_{\Sigma^{-1}}'$ on $\mathbb{R}^d$. To verify that (2.4.2) holds with the stated values of β, Λ, first fix $x \in \mathbb{R}^d$. The bound (2.4.2) holds trivially if $\nabla f(x) = 0$, so we may assume that $\nabla f(x) \neq 0$. Let $u := -\Sigma\,\nabla f(x)$, and for $t \in \mathbb{R}$, let

$h(t) := f(x+tu)$. By the chain rule, we have $h'(t) = \nabla f(x+tu)^\top u$ for all $t \in \mathbb{R}$, so upon applying the Cauchy–Schwarz inequality and the defining condition (2.4.6) for the class $\mathcal{H}^{\beta,L}$, it follows that

$$\begin{aligned} |h'(t) - h'(s)| &= |\{\nabla f(x+tu) - \nabla f(x+su)\}^\top u| \\ &= (\det \Sigma)^{-1} \langle \nabla f(x+tu) - \nabla f(x+su), \Sigma^{-1} u\rangle' \\ &\leq (\det \Sigma)^{-1} \|\nabla f(x+tu) - \nabla f(x+su)\|'_{\Sigma^{-1}} \|\Sigma^{-1}u\|'_{\Sigma^{-1}} \\ &\leq (\det \Sigma)^{-1} L \|(t-s)u\|_\Sigma^{\beta-1} \|\nabla f(x)\|'_{\Sigma^{-1}} \\ &= (\det \Sigma)^{-(\beta+1)/2} L|t-s|^{\beta-1} (\|\nabla f(x)\|'_{\Sigma^{-1}})^\beta \end{aligned}$$

for all $t, s \in \mathbb{R}$. Hence, writing $\lambda := (\det \Sigma)^{-1/2} \|\nabla f(x)\|'_{\Sigma^{-1}}$, we deduce that

$$h'(t) \leq h'(0) + Lt^{\beta-1}\lambda^\beta (\det \Sigma)^{-1/2} = -\lambda^2 + Lt^{\beta-1}\lambda^\beta (\det \Sigma)^{-1/2}$$

for all $t \geq 0$. Since h takes non-negative values, we can apply the fundamental theorem of calculus to see that

$$\begin{aligned} -f(x) = -h(0) \leq h(t) - h(0) &= \int_0^t h'(s)\, ds \\ &\leq \int_0^t \left\{-\lambda^2 + Ls^{\beta-1}\lambda^\beta (\det\Sigma)^{-1/2}\right\} ds \\ &= (\det \Sigma)^{-1/2} \left\{-\|\nabla f(x)\|'_{\Sigma^{-1}} (\lambda t) + \frac{L}{\beta} (\lambda t)^\beta\right\} =: G(\lambda t) \end{aligned}$$

for all $t \geq 0$. We now optimise this bound by setting $t = a^*/\lambda$, where $a^* := \operatorname{argmin}_{t\geq 0} G(t) = (\|\nabla f(x)\|'_{\Sigma^{-1}}/L)^{1/(\beta-1)}$, which yields

$$f(x) \geq -G(a^*) = (\det \Sigma)^{-1/2} (1 - 1/\beta)\, L^{-1/(\beta-1)} (\|\nabla f(x)\|'_{\Sigma^{-1}})^{\beta/(\beta-1)}.$$

This establishes the desired bound (2.4.2) on $\|\nabla f(x)\|'_{\Sigma^{-1}}$, and in view of Proposition 2.4.2, the final assertion of (i) now follows immediately. Observe in particular that, in addition to the defining condition (2.4.6), the key property of $f \in \mathcal{H}^{\beta,L}$ that we exploit in the argument above is the non-negativity of f. Since we do not appeal to the log-concavity of f or even the fact that f is a density, we may therefore run through the same proof with Σ replaced by I throughout in order to establish (ii) for general non-negative functions $g\colon \mathbb{R}^d \to [0,\infty)$ that satisfy $\|\nabla g(y) - \nabla g(x)\| \leq L\|y-x\|^{\beta-1}$ for all $x, y \in \mathbb{R}^d$.

For (iii), since $\mathcal{H}^{\beta,L}$ is affine invariant (cf. Example 2.5 in the main text and Lemma 2.8.5), it suffices to consider $f \in \mathcal{H}^{\beta,L} \cap \mathcal{F}^{0,I}$. To verify that (2.4.2) holds with the stated values of β, Λ, fix $x \in \mathbb{R}^d$ with $\nabla f(x) \neq 0$, and let $u := -\nabla f(x)/\|\nabla f(x)\|$. Note that by the log-concavity of the density f, the function $h\colon [0,\infty) \to [0,\infty)$ defined by $h(t) := f(x+tu)$ is strictly decreasing and non-negative. Using the chain rule, we find that $h'(t) = \nabla f(x+tu)^\top u$ and $h''(t) = u^\top Hf(x+tu)u$ for all t, and it follows from the defining condition (2.4.7) for the class $\mathcal{H}^{\beta,L}$ that

$$\begin{aligned} |h''(t) - h''(s)| &= |u^\top \{Hf(x+tu) - Hf(x+su)\}u| \\ &\leq \|Hf(x+tu) - Hf(x+su)\|_{\mathrm{F}} \leq L|t-s|^{\beta-2} \end{aligned}$$

for all $t, s \geq 0$. Therefore, recalling that h is decreasing, we now apply the fundamental theorem of calculus to deduce that

$$\begin{aligned}-h'(0) \geq h'(t) - h'(0) &= \int_0^t h''(s)\,ds \\ &\geq \int_0^t \big(h''(0) - Ls^{\beta-2}\big)\,ds = h''(0)t - \frac{L}{\beta-1}t^{\beta-1},\end{aligned}$$

for all $t \geq 0$. Setting $\lambda := \|\nabla f(x)\| = -h'(0)$ and $\tilde{\Lambda} := \Lambda(\beta-1, L)$, as defined in (i), we now optimise this bound with respect to t as in the proof of (i) and conclude that $h''(0) \leq \tilde{\Lambda}\lambda^{(\beta-2)/(\beta-1)}$. On the other hand, we have

$$h'(t) - h'(0) = \int_0^t h''(s)\,ds \leq \int_0^t \big(h''(0) + Ls^{\beta-2}\big)\,ds = h''(0)t + \frac{L}{\beta-1}t^{\beta-1},$$

for all $t \geq 0$, and a further application of the fundamental theorem of calculus yields

$$\begin{aligned}h(t) - h(0) \leq \int_0^t h'(s)\,ds &\leq \int_0^t \Big(h'(0) + h''(0)s + \frac{L}{\beta-1}s^{\beta-1}\Big)\,ds \\ &\leq -\lambda t + \frac{\tilde{\Lambda}}{2}\lambda^{(\beta-2)/(\beta-1)}\,t^2 + \frac{L}{\beta(\beta-1)}t^{\beta}\end{aligned}$$

for all $t \geq 0$. Replacing t by $\lambda^{1/(\beta-1)}t$ and using the fact that $h \geq 0$, we see that

$$0 \leq h(0) - \Big(t - \frac{\tilde{\Lambda}}{2}t^2 - \frac{L}{\beta(\beta-1)}t^{\beta}\Big)\,\lambda^{\beta/(\beta-1)} =: h(0) - \alpha(t)\lambda^{\beta/(\beta-1)}$$

for all $t \geq 0$. Letting $\tilde{\alpha} := \max_{t \geq 0} \alpha(t) > 0$, we deduce that $\|\nabla f(x)\| = \lambda \leq \{\tilde{\alpha}^{-1}h(0)\}^{1-1/\beta} = \{\tilde{\alpha}^{-1}f(x)\}^{1-1/\beta}$. Since $\tilde{\alpha}$ depends only on β and L, the proof of (iii) is complete.

Finally, in view of the affine invariance of the conditions (2.4.2), (2.4.4), (2.4.5), it suffices to prove assertion (iv) for $f \in \mathcal{F}^{0,I} \cap \tilde{\mathcal{H}}^{\gamma,L}$. We begin by recalling that there exists $\tilde{B} \equiv \tilde{B}_d > 0$ such that $h(x) \leq e^{\tilde{B}_d}$ for all $h \in \mathcal{F}_d^{0,I}$ and $x \in \mathbb{R}^d$, (e.g. Kim and Samworth, 2016, Theorem 2(a)). Consequently, if $f \in \mathcal{F}^{0,I} \cap \tilde{\mathcal{H}}^{\gamma,L}$, then the function $\psi\colon \mathbb{R}^d \to \mathbb{R}$ defined by $\psi(x) = -\log f(x) + \tilde{B}$ is (γ, L)-Hölder and takes non-negative values. Thus, if $x, y \in \mathbb{R}^d$ satisfy $f(y) < f(x) < e^{-1}$ and if $\beta > 1$, then

$$\begin{aligned}\|x-y\| \geq \Lambda(\gamma,L)^{-1}\,\frac{\psi(y)-\psi(x)}{\psi(y)^{1-1/\gamma}} &= \Lambda(\gamma,L)^{-1}\,\frac{\log f(x) - \log f(y)}{\{\log\{1/f(y)\} + \tilde{B}\}^{1-1/\gamma}} \\ &\geq (\tilde{B}+1)^{-1}\,\Lambda(\gamma,L)^{-1}\,\frac{\log f(x) - \log f(y)}{\log\{1/f(y)\}} \\ &\geq (\tilde{B}+1)^{-1}\,\Lambda(\gamma,L)^{-1}\,\beta^{-1}\,\frac{f(x)-f(y)}{f(x)^{1-1/\beta}},\end{aligned}$$

where we applied assertion (ii) of the proposition and Lemma 2.8.8 below to obtain the first and last inequalities in the display above. This yields the first assertion of (iv). Since $\Lambda(\gamma, L)$ is bounded above by $(L \vee L^{1/2})\max_{0<w\leq 1/2} w^{-w} = (L \vee L^{1/2})\,e^{1/e}$ for all $\gamma \in (1,2]$, the final conclusion of (iv) follows immediately upon setting $\tau = e^{-1}$ and invoking Proposition 2.4.1(ii). □

The following simple bound is used in the proof of Proposition 2.8.7(iii).

Lemma 2.8.8. *If $\beta \geq 1$ and $0 < a < b < 1$, then*

$$\frac{\log b - \log a}{\log (1/a)} > \frac{\beta^{-1}(b-a)}{b^{1-1/\beta}}. \tag{2.8.16}$$

Proof. Setting $u := \log(e^\beta/b)$, we can differentiate the function $w \mapsto we^{1-w/\beta}$ to deduce that

$$b^{1/\beta}\log(e^\beta/b) = ue^{1-u/\beta} < \beta \tag{2.8.17}$$

for all $b \in (0,1)$. Now fix $b \in (0,1)$ and suppose first that $a \in [be^{-\beta}, b]$. By the mean value theorem, there exists $c \in (a,b)$ such that $(\log b - \log a)/(b-a) = 1/c$, and it follows from (2.8.17) that

$$\frac{\log b - \log a}{b-a} = \frac{1}{c} \geq \frac{1}{b} > \frac{\beta^{-1}\log(e^\beta/b)}{b^{1-1/\beta}} \geq \frac{\beta^{-1}\log(1/a)}{b^{1-1/\beta}},$$

so (2.8.16) holds when $a \in [be^{-\beta}, b]$. On the other hand, when $a \in (0, be^{-\beta})$, note that the left-hand side of (2.8.16) is a decreasing function of a for each fixed value of b. Thus, we see that

$$\frac{\log b - \log a}{\log (1/a)} \geq \frac{\beta}{\log(e^\beta/b)} \geq b^{1/\beta} > \frac{\beta^{-1}(b-a)}{b^{1-1/\beta}},$$

as required, where we have again used (2.8.17) to obtain the second inequality above. □

Review of results on nonparametric density estimation over Hölder classes

When $d = 3$, $\beta \in (1,2]$ and $L > 0$, we saw in Example 2.5 that $\sup_{f_0 \in \mathcal{H}_d^{\beta,L}} \mathbb{E}_{f_0}\{d_X^2(\hat{f}_n, f_0)\} \lesssim_{\beta,L} n^{-(\beta+3)/(\beta+7)} \log^{\lambda_\beta} n$, where $\lambda_\beta := (16\beta + 39)/(2(\beta+7))$. To relate this result to the existing literature on nonparametric density estimation over Hölder classes of densities (without shape constraints), we work with d_{H}^2 instead of d_X^2 divergence (since the latter is specific to the estimator $\hat{f}_n$), and borrow some definitions from Goldenshluger and Lepski (2014). For $d \in \mathbb{N}$, let $\mathbf{1}_d := (1,\ldots,1) \in \mathbb{R}^d$, and for $\beta \in (1,2]$ and $L > 0$, denote by $\mathcal{H}(\beta, L) \equiv \mathcal{H}_d(\beta, L)$ the anisotropic Nikol'skii class $\mathcal{N}_{\infty\mathbf{1}_d,d}(\beta\mathbf{1}_d, L\mathbf{1}_d) = \mathcal{N}_{\infty\mathbf{1}_d,d}(\beta\mathbf{1}_d, L\mathbf{1}_d, L)$ of densities $g\colon \mathbb{R}^d \to \mathbb{R}$ satisfying $|g(x)| \leq L$ and $|g(x+2h) - 2g(x+h) + g(x)| \leq L\|h\|^\beta$ for all $x, h \in \mathbb{R}^d$; see (3.2) on page 488 of Goldenshluger and Lepski (2014). This is slightly different to our Hölder conditions (2.4.6) and (2.8.10), but with the aid of Taylor's theorem (with the mean value form of the remainder) and Proposition 2.8.6, we can verify that whenever $\beta \in (1,2]$ and $L > 0$, there exists $L' \equiv L'(d,\beta,L) > 0$ such that $\mathcal{H}^{\beta,L} \subseteq \mathcal{H}(\beta, L')$.

Recalling the standard fact that $d_{\mathrm{H}}^2(f,g) \geq \|f-g\|_1^2/4 = (\int_{\mathbb{R}^d} |f-g|)^2/4$ for all densities f, g, we can apply the Cauchy–Schwarz inequality and take $p = 1$ in Goldenshluger and Lepski (2014, Theorem 3(i)) to deduce that there exists $c \equiv c(\beta, d) > 0$ such that

$$\inf_{\tilde{f}_n} \sup_{f_0 \in \mathcal{H}(\beta,L')} \mathbb{E}_{f_0}\{d_{\mathrm{H}}^2(\tilde{f}_n, f_0)\} \geq \inf_{\tilde{f}_n} \sup_{f_0 \in \mathcal{H}(\beta,L')} \mathbb{E}_{f_0}\{\|\tilde{f}_n - f_0\|_1\}^2/4 \geq c > 0, \tag{2.8.18}$$

where the infimum is taken over all estimators $\tilde{f}_n$ based on n observations. In other words, it is not even possible to achieve consistency over $\mathcal{H}(\beta, L')$ with respect to L^1 (and hence d_{H}^2) loss. In view of this, it will be more meaningful to compare the result of Example 2.5 with (a lower bound on) the minimax d_{H}^2 risk over a carefully chosen subclass of $\mathcal{H}(\beta, L')$.

Suppose henceforth that $d = 3$, and for fixed $\beta \in (1,2]$ and $L > 0$, let $L' \equiv L'(3,\beta,L) > 0$ and $\mathcal{H}(\beta, L') \equiv \mathcal{H}_3(\beta, L')$ be as above. In the notation of Goldenshluger and Lepski (2014, Sections 3.3 and 4), the parameters associated with this class are $\beta_1 = \beta_2 = \beta_3 = \beta$ and $s = \infty$, and to avoid confusion, we write $\tilde{\beta}$ for the quantity $\bigl(\sum_{j=1}^d \beta_j^{-1}\bigr)^{-1} = \beta/d = \beta/3$ that these authors denote by β.

By Example 2.5 and the affine invariance of d_{H}^2, we have

$$\sup_{f_0 \in \mathcal{H}^{\beta,L} \cap \mathcal{F}^{0,I}} \mathbb{E}_{f_0}\{d_{\mathrm{H}}^2(\hat{f}_n, f_0)\} = \sup_{f_0 \in \mathcal{H}^{\beta,L}} \mathbb{E}_{f_0}\{d_{\mathrm{H}}^2(\hat{f}_n, f_0)\} \lesssim_{\beta,L} n^{-(\beta+3)/(\beta+7)} \log^{\lambda_\beta} n. \tag{2.8.19}$$

We now show that $\mathcal{H}^{\beta,L} \cap \mathcal{F}^{0,I}$ is contained within a subclass of $\mathcal{H}(\beta, L')$ over which the minimax L^1 risk is $\tilde{O}(n^{-2\beta/(2\beta+3)})$, rather than of constant order as in (2.8.18). The key fact we exploit is that $\mathcal{F}^{0,I}$ has an envelope function that decays exponentially in the following sense. For $a > 0$ and $b \in \mathbb{R}$, denote by $\mathcal{G}(a,b)$ the set of $g \colon \mathbb{R}^3 \to \mathbb{R}$ such that $g(x) \leq e^{-a\|x\|+b}$ for all $x \in \mathbb{R}^3$, and recall that there exist universal constants $A > 0$ and $B \in \mathbb{R}$ such that $\mathcal{G}(A,B) \supseteq \mathcal{F}^{0,I} \equiv \mathcal{F}_3^{0,I}$ (e.g. Kim and Samworth, 2016, Theorem 2(a)). Now for $g \in \mathcal{G}(a,b)$, define $g^* : \mathbb{R}^3 \to [0,\infty)$ as in (4.1) on page 493 of Goldenshluger and Lepski (2014), so that $g^*(x) := \sup_{H_x} \mu_3(H_x)^{-1} \int_{H_x} g$ for each $x \in \mathbb{R}^3$, where the supremum is taken over all hyperrectangles H_x of the form $\prod_{j=1}^3 [x_j - h_j/2,\, x_j + h_j/2]$ with $h_1, h_2, h_3 \in (0,2]$. Then $g^*(x) \leq \sup_{h \in [-1,1]^3} g(x+h) \leq \sup_{h \in [-1,1]^3} e^{-a\|x+h\|+b} \leq e^{-a\|x\|+(a\sqrt{3}+b)}$ for all $x \in \mathbb{R}^3$. Setting $\theta \equiv \theta(\beta) := 1/(2+1/\tilde{\beta}) = \beta/(2\beta+3) \in (0,1)$, we deduce that there exists $R = R(a,b,\beta) > 0$ such that every $g \in \mathcal{G}(a,b)$ satisfies the 'tail dominance' condition $\bigl(\int_{\mathbb{R}^3} (g^*)^\theta\bigr)^{1/\theta} \leq R$, which is the defining property (4.2) of the class $\mathcal{G}_\theta(R)$ on page 493 of Goldenshluger and Lepski (2014). Therefore, $\mathcal{F}^{0,I} \subseteq \mathcal{G}(A,B) \subseteq \mathcal{G}_\theta(R')$, where $R' := R(A,B,\beta)$.

Recall that $s = \infty$ and that our $\tilde{\beta} = \beta/3$ corresponds to the parameter β in their notation, so that $\nu^*(\theta) = 1/(2+1/\tilde{\beta}) = \beta/(2\beta+3)$ in the last display on page 493 of Goldenshluger and Lepski (2014). Consequently, by taking $p = 1$ in Goldenshluger and Lepski (2014, Theorem 4(i)), we deduce that there exists $R'' \equiv R''(\beta, L) > 0$ such that

$$\inf_{\tilde{f}_n} \sup_{f_0 \in \mathcal{H}(\beta,L') \cap \mathcal{G}_\theta(\tilde{R})} \mathbb{E}_{f_0}\{d_{\mathrm{H}}^2(\tilde{f}_n, f_0)\} \geq \inf_{\tilde{f}_n} \sup_{f_0 \in \mathcal{H}(\beta,L') \cap \mathcal{G}_\theta(\tilde{R})} \mathbb{E}_{f_0}\{\|\tilde{f}_n - f_0\|_1\}^2/4 \gtrsim_{\beta,L} n^{-2\beta/(2\beta+3)} \tag{2.8.20}$$

for all $\tilde{R} \geq R''$, where the first inequality follows as in (2.8.18) and the second inequality is tight up to logarithmic factors by Remark 3(4) on page 495 of Goldenshluger and Lepski (2014). Since $\mathcal{H}^{\beta,L} \cap \mathcal{F}^{0,I} \subseteq \mathcal{H}(\beta, L') \cap \mathcal{G}_\theta(R' \vee R'')$, the minimax lower bound in (2.8.20) suggests that under the assumption of log-concavity, it is possible to achieve faster rates of convergence at least when $\beta \in (1, 9/5)$. However, this does not rule out the possibility that these accelerated rates could be obtained under a weaker exponential tail condition in place of the stronger constraint of log-concavity. To show that this is not the case, we observe that the proof of (2.8.20) considers only a subset of densities in $\mathcal{H}(\beta, L') \cap \mathcal{G}_\theta(R')$ whose supports are contained within $[-N, N]^3$ for some $N \equiv N(\beta, L) > 0$. There exist $a' \equiv a'(\beta, L) \in (0, A]$ and $b' \equiv b'(\beta, L) \geq B$ such that all such densities are contained within $\mathcal{G}(a', b')$, so we actually have

$$\inf_{\tilde{f}_n} \sup_{f_0 \in \mathcal{H}(\beta,L') \cap \mathcal{G}(a',b')} \mathbb{E}_{f_0}\{d_{\mathrm{H}}^2(\tilde{f}_n, f_0)\} \geq \inf_{\tilde{f}_n} \sup_{f_0 \in \mathcal{H}(\beta,L') \cap \mathcal{G}(a',b')} \mathbb{E}_{f_0}\{\|\tilde{f}_n - f_0\|_1\}^2/4 \gtrsim_{\beta,L} n^{-2\beta/(2\beta+3)}. \tag{2.8.21}$$

Since $\mathcal{H}^{\beta,L} \cap \mathcal{F}^{0,I} \subseteq \mathcal{H}(\beta, L') \cap \mathcal{G}(A,B) \subseteq \mathcal{H}(\beta, L') \cap \mathcal{G}(a', b')$, we may justifiably conclude on the basis of (2.8.19) and (2.8.21) that the improvement in the rates attainable is indeed due to the log-concavity shape constraint rather than the exponential tail decay exhibited by log-concave densities.

Chapter 3

Estimation of S-shaped functions

We define a function $f\colon [0,1] \to \mathbb{R}$ to be *S-shaped* if it is increasing, and if there exists $m_0 \in [0,1]$ such that f is convex on $[0, m_0]$ and concave on $[m_0, 1]$. The point m_0 is called an *inflection point*, and we do not insist that f is continuous at m_0; the cases $m_0 = 0$ and $m_0 = 1$ correspond to increasing concave and increasing convex functions respectively. Various examples of S-shaped functions are shown in Figure 3.1. In many areas of applied science, there are domain-specific reasons to model the regression of a response variable on a covariate as an S-shaped function. For instance, development curves for individuals or populations often exhibit S-shaped behaviour in the context of biological growth (Archontoulis and Miguez, 2015; Cao et al., 2019; Zeidi, 1993) or skill proficiency (Gibbs, 2000). Further examples where time is the covariate can be found in audio signal processing (Smith, 2010) and sociology (Tarde, 1903). In agronomy, the van Genuchten–Gupta model (van Genuchten and Gupta, 1993) postulates an inverted S-shaped relationship between crop yield and soil salinity, and S-shaped trends are also observed for the production levels of commercial goods as labour or other resources are scaled up (Ginsberg, 1974). For the latter, economic principles such as the Regular Ultra Passum law (Frisch, 1964) have been formulated to describe scenarios where marginal gains (i.e. returns to scale) increase up to a point of maximal productivity and then taper off.

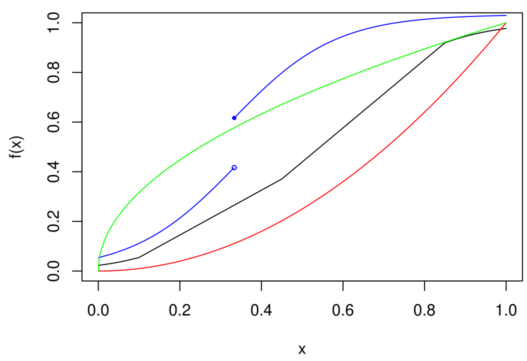

Figure 3.1: Some examples of S-shaped functions on $[0, 1]$.

In some of the examples above, for instance when population or disease dynamics can be modelled by some governing differential equation, it may be natural to confine attention to certain parametric subclasses of S-shaped functions, such as those consisting of sigmoidal (i.e. logistic) functions of the form

$$f(x; A, a, b) = \frac{A}{1 + e^{-ax+b}}, \tag{3.0.1}$$

with $A, a > 0$ and $b \in \mathbb{R}$; see also Jarne et al. (2007). However, in many other settings, such domain-specific knowledge is often lacking, and parametric assumptions may be excessively restrictive. To illustrate this effect, see Figure 3.2, where we compare two popular parametric fits of an S-shaped regression function with the estimator we propose in this chapter. The first parametric method fits a logistic curve of the form (3.0.1) using nonlinear least squares. The second uses segmented linear regression with two kinks, fitted using least squares and a search over the locations of the kinks. Although these parametric fits appear to the naked eye to be satisfactory, it turns out that their estimation performance, as measured by the squared error loss on the training data, is roughly six times worse than that of our proposal (on average 0.38 and 0.43 compared with 0.067, over 100 repetitions). If the noise standard deviation is halved, then these parametric methods become 17 times and 19 times worse than our proposal respectively.

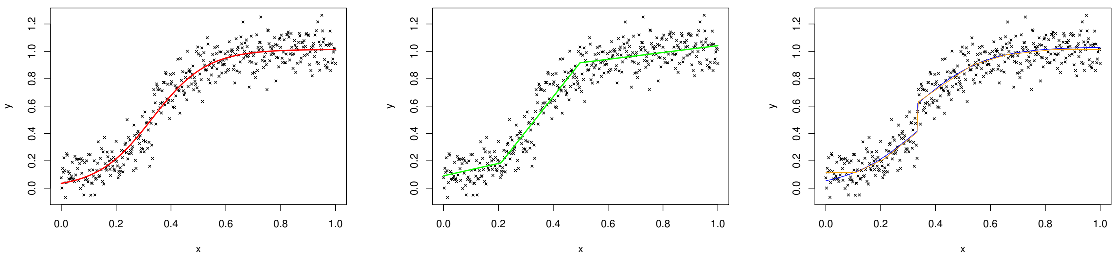

Figure 3.2: Logistic (red, left), segmented linear regression (green, middle) and our S-shaped estimator (orange, right) of the true regression function given in blue on the right.

Motivated by the limitations described in the previous paragraph, the goal of this chapter is to introduce a flexible framework for nonparametric estimation of S-shaped functions. The main challenges in removing the parametric restrictions are two-fold: first, the class $\mathcal{F}$ of S-shaped functions on $[0, 1]$ is infinite-dimensional; and second, since the inflection point is unknown, the family $\mathcal{F}$ is non-convex. In spite of this non-convexity, we are able to develop methodology based on L^2-projections of general distributions onto $\mathcal{F}$. The significant advantage of working in this additional generality is that, having established continuity properties of the projection, results on the consistency and robustness under misspecification of the estimator follow as simple corollaries of basic facts about convergence of empirical distributions. Nevertheless, since the fully general statements are fairly involved, we defer this formal presentation to Section 3.5.4, and focus in Section 3.1 on the special case of projections of the empirical distribution of data of the form $(x_1, Y_1), \ldots, (x_n, Y_n) \in [0, 1] \times \mathbb{R}$ with $x_1 < \cdots < x_n$. This allows us to prove that an S-shaped least squares estimator always exists, and to study its uniqueness properties. Moreover, when the design is fixed and the errors are independent and identically distributed with mean zero and finite variance, we present a basic consistency result that follows from the general theory in Section 3.5.4.

In Section 3.2, we take up the challenge of computing the S-shaped least squares estimator. Since its inflection point occurs at one of the design points, a naive strategy would be to fit, for each choice of $m \in \{x_1, \ldots, x_n\}$, the least squares estimate over the class of S-shaped functions with inflection point m, before selecting a solution that minimises the residual sum of squares. The individual constrained estimates are straightforward to compute using, e.g., active set methods (Dümbgen et al., 2007; Nocedal and Wright, 2006, Chapters 12 and 16.5), but it can be time-consuming to run the active set method n times. We show how a simple refinement of the search strategy can improve the running time by a factor of around 4, but our major contribution here begins with the observation that the global S-shaped least squares estimate can be obtained as a concatenation of a convex increasing least squares estimate to the left of an estimated inflection point, with a concave increasing least squares estimate to the right. This enables us to pursue a sequential approach, where we reveal new observations one by one, and update the least squares fits using a mixed primal-dual bases algorithm (Fraser and Massam, 1989; Meyer, 1999). Our algorithm, which is available in the `R` package `Sshaped` (Feng et al., 2021c), is shown to be around 40 times faster than the naive strategy in examples; see Figure 3.5.

Our main theoretical contributions are presented in Section 3.3, under an independent and sub-Gaussian error assumption. Here, we derive worst-case and adaptive sharp oracle inequalities for the S-shaped least squares estimator. When combined with our corresponding minimax lower bounds, this theory reveals in particular that the S-shaped least squares estimator attains the optimal worst-case risk of order $n^{-2/5}$ with respect to L^2-loss, in the case where the design points are not too irregularly spaced. These results apply both when the S-shaped regression function hypothesis is correctly specified, and where it is misspecified, provided in the latter case that we interpret the loss as the distance to the projection of the signal onto $\mathcal{F}$. For adversarially-chosen design configurations, we show that the risk bound can deteriorate to $n^{-1/3}$ in the worst case. Moreover, the S-shaped least squares estimator adaptively attains the parametric rate of order $n^{-1/2}$ (up to a logarithmic factor), when the projection of the signal is piecewise affine with a relatively small number of affine pieces. Finally, we study the delicate problem of estimating the true inflection point m_0, which represents the boundary between the convex and concave parts of the signal. Under an appropriate local smoothness assumption indexed by a parameter $\alpha > 0$, we show that the inflection point $\hat{m}_n$ of the least squares estimator converges to m_0 at rate $O_p\big((n^{-1}\log n)^{1/(2\alpha+1)}\big)$, which matches our local asymptotic minimax lower bound, up to the logarithmic factor. Interestingly, the combination of the monotonicity with the convexity/concavity means that our S-shaped estimator is sufficiently regularised to avoid boundary problems at the endpoints $\{0, 1\}$ of the covariate domain; other common shape constrained methods are known to lead to boundary estimation inconsistency (Balabdaoui et al., 2011; Balász et al., 2015; Cule et al., 2010; Kulikov and Lopuhaä, 2006; Samworth, 2018).

In Section 3.4, we study the empirical properties of our S-shaped least squares estimator, comparing both its running time and statistical performance with those of alternative approaches. In Section 3.5, we give the proofs of our main results, and also derive some 'subinterval localisation' results for univariate shape-constrained estimators, which may be of independent interest. Moreover, we provide further details of the mixed primal-dual bases algorithm that we use to compute our estimator. Several auxiliary results and derivations are deferred to Section 3.6.

Previous work on nonparametric estimation of S-shaped functions includes Yagi et al. (2019, 2020), who, in the context of production theory in economics, apply a method known as shape constrained kernel least squares to estimate multivariate production functions that are S-shaped along one-dimensional rays. Kachouie and Schwartzman (2013) use local polynomial regression techniques to identify an inflection point of a smooth signal from corrupted observations. In both of these works, kernel bandwidths must be chosen carefully to control the bias-variance tradeoff and (for the approach of Kachouie and Schwartzman (2013) in particular) to ensure that the fitted curve does not have multiple inflection points. Liao and Meyer (2017) instead estimate univariate convex-concave functions using cubic splines defined with respect to a number of user-specified knots, and establish rates of convergence for the inflection points of the resulting estimators. We also mention the extremum distance estimator and extremum surface estimator proposed by Christopoulos (2016), with the aim of locating the inflection point of a smooth function based on its geometric properties. We provide a numerical comparison of our procedure with those of Liao and Meyer (2017), Yagi et al. (2019, 2020) and Christopoulos (2016) in Section 3.4.2.

3.1 Existence, uniqueness and consistency of S-shaped least squares estimators

The purpose of this section is to study the existence, uniqueness and consistency of S-shaped least squares estimators. We will see later that these estimators can be regarded as the L^2-projection onto $\mathcal{F}$ of the empirical distribution of our data $(x_1, Y_1), \dots, (x_n, Y_n)$. As such, the results in this section turn out to be special cases of a much more general theory, presented in Section 3.5.4, concerning the existence and continuity of L^2-projections of arbitrary distributions on $[0,1] \times \mathbb{R}$ having finite variance. The generality of this projection framework remains of importance to statisticians, particularly in terms of providing results on the robustness of S-shaped least squares estimators to model misspecification; however, the results are of a more technical nature, so to facilitate understanding of the main ideas, we focus on the well-specified case here.

For each $m \in [0,1]$, we let $\mathcal{F}^m$ denote the class of functions $f\colon [0,1] \to \mathbb{R}$ that are convex on $[0,m]$, concave on $[m,1]$ and increasing (i.e. non-decreasing) on $[0,1]$. Thus $\mathcal{F} = \bigcup_{m \in [0,1]} \mathcal{F}^m$, but this union of convex sets is not itself convex. Suppose we have data $(x_1, Y_1), \dots, (x_n, Y_n) \in [0,1] \times \mathbb{R}$ with $x_1 < \dots < x_n$. If $\tilde{f}_n\colon [0,1] \to \mathbb{R}$ minimises* $f \mapsto \sum_{i=1}^n \bigl(Y_i - f(x_i)\bigr)^2 =: S_n(f)$ over some class $\tilde{\mathcal{F}}$ of functions on $[0,1]$, we say that $\tilde{f}_n$ is a *least squares estimator (LSE) over* $\tilde{\mathcal{F}}$ based on $\{(x_i, Y_i) : 1 \le i \le n\}$.

Proposition 3.1.1. *For each $m \in [0,1]$, there exists an LSE $\tilde{f}_n^m$ over $\mathcal{F}^m$ that is uniquely determined at $x_1, \dots, x_n$. Moreover, there exists an LSE $\tilde{f}_n$ over $\mathcal{F}$ with an inflection point in $\{x_1, \dots, x_n\}$.*

Proposition 3.1.1 is a consequence of Corollary 3.5.13(d) in Section 3.5.4. Since our objective criterion only measures the error incurred at the design points, it is no surprise that any LSE $\tilde{f}_n^m$ over $\mathcal{F}^m$ can only be unique at $x_1, \dots, x_n$. There is a canonical way to define $\tilde{f}_n^m$ on the whole of $[0,1]$, namely by linear interpolation between its kinks. Thus, the slope remains constant on $[0, x_2], [x_2, x_3], \dots, [x_{n-2}, x_{n-1}], [x_{n-1}, 1]$, and we denote this interpolating function by $\hat{f}_n^m$. A subtle issue, however, is that when m is not a design point, $\hat{f}_n^m$ need not belong to $\mathcal{F}^m$; see the left panel of Figure 3.3. To finesse this point, let $\mathcal{G} \equiv \mathcal{G}[x_1, \dots, x_n]$ denote the set of continuous, piecewise affine $f\colon [0,1] \to \mathbb{R}$ with kinks in $\{x_2, \dots, x_{n-1}\}$ and, for $m \in [0,1]$, denote by $\mathcal{H}^m \equiv \mathcal{H}^m[x_1, \dots, x_n]$ the class of all $f \in \mathcal{G}$ for which there exists $g \in \mathcal{F}^m$ with $f = g$ on $\{x_1, \dots, x_n\}$. Then $\mathcal{H}^m$ is a closed, convex cone, and the LSE over $\mathcal{H}^m$ based on $\{(x_i, Y_i) : 1 \le i \le n\}$ is precisely the function $\hat{f}_n^m$. We refer to $\hat{f}_n^0$ and $\hat{f}_n^1$ as the *increasing concave* LSE and *increasing convex* LSE (based on $\{(x_i, Y_i) : 1 \le i \le n\}$) respectively.

It turns out, however, that in general an LSE $\tilde{f}_n$ over $\mathcal{F}$ is not even uniquely defined at the design points. For instance, if our data are $(0,0), (1/3, 1/2), (2/3, 1/2), (1,1)$, then the linear interpolations of both $(0,0), (1/3, 5/12), (2/3, 2/3), (1, 11/12)$ and $(0, 1/12), (1/3, 1/3), (2/3, 7/12), (1,1)$ are LSEs over $\mathcal{F}$; see the right panel of Figure 3.3. We remark that this non-uniqueness is not related to the small number of data points, but rather to the symmetry of the data configuration.

In order to present a basic consistency result, we introduce a model where we regard our data $\{(x_1, Y_1), \dots, (x_n, Y_n)\} \equiv \{(x_{n1}, Y_{n1}), \dots, (x_{nn}, Y_{nn})\}$ as being realised from a triangular array sampling scheme

$$Y_{ni} = f_0(x_{ni}) + \xi_{ni}, \quad i = 1, \dots, n, \tag{3.1.1}$$

where $f_0\colon [0,1] \to \mathbb{R}$ is a Borel measurable regression function, where $\xi_{n1}, \dots, \xi_{nn}$ are independent and identically distributed noise variables with mean zero and finite variance, and where $0 \le x_{n1} <$

*Since there may be multiple minimisers, we will also assume throughout and without further comment that $\tilde{f}_n$ is chosen to depend measurably on $(x_1, Y_1), \dots, (x_n, Y_n)$. Likewise, we will assume the same property for estimated inflection points.

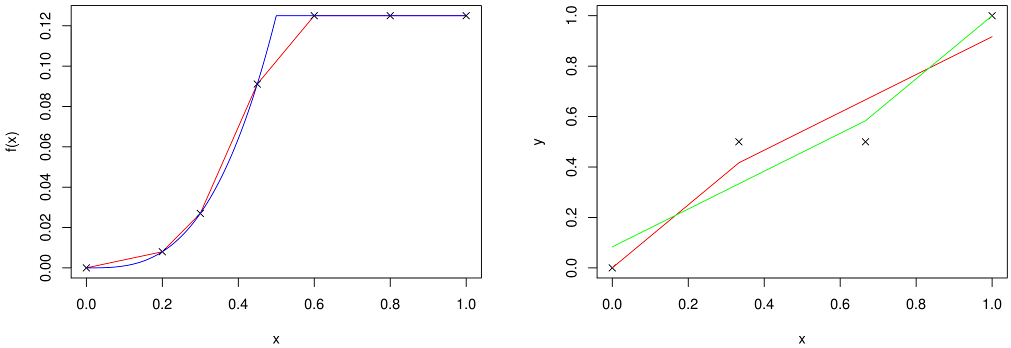

Figure 3.3: Left: For noiseless observations of the blue regression function at the black crosses, the red curve illustrates the linear interpolation $\hat{f}_n^m$ of the LSE, with $m = 0.5$; here, the segment of steepest slope does not contain $x = 0.5$, so $\hat{f}_n^m$ does not belong to $\mathcal{F}^m$ with $m = 0.5$. Right: For the data given by the black crosses, both the red curve and the green curve are LSEs over $\mathcal{F}$.

$\cdots < x_{nn} \leq 1$ are fixed design points. We write $\mathbb{P}_n := n^{-1}\sum_{i=1}^n \delta_{(x_{ni},Y_{ni})}$ and $\mathbb{P}_n^X := n^{-1}\sum_{i=1}^n \delta_{x_{ni}}$ for the joint and X-marginal empirical distributions respectively.

For a finite Borel measure ν on $[0,1]$, we write $\operatorname{supp}\nu$ for the *support* of ν, which is defined as the smallest closed set A such that $\nu(A^c) = 0$, or equivalently the set of all $x \in [0,1]$ with the property that $\nu(U) > 0$ for any open neighbourhood U of x in $[0,1]$.

Proposition 3.1.2. *In model (3.1.1), assume that $f_0 \in \mathcal{F}$ has unique inflection point $m_0 \in [0,1]$. For each $n \in \mathbb{N}$, let $\hat{f}_n^{m_0}$ and $\tilde{f}_n$ denote LSEs over $\mathcal{F}^{m_0}$ and $\mathcal{F}$ respectively. Suppose further that $(\mathbb{P}_n^X)$ converges weakly to a distribution P_0^X on $[0,1]$ satisfying $\operatorname{supp} P_0^X = [0,1]$ and $P_0^X(\{m\}) = 0$ for all $m \in [0,1]$. Then, for $\tilde{g}_n \in \{\hat{f}_n^{m_0}, \tilde{f}_n\}$ and with $\tilde{m}_n$ denoting any inflection point of $\tilde{g}_n$, we have*

(a) $\tilde{m}_n \xrightarrow{p} m_0$;

(b) $\sup_{x\in A} |(\tilde{g}_n - f_0)(x)| \xrightarrow{p} 0$ *for any closed set* $A \subseteq [0,1] \setminus \{m_0\}$;

(c) If $m_0 \in (0,1)$, *then* $\int_0^1 |\tilde{g}_n - f_0|^q \, dP_0^X \xrightarrow{p} 0$ *for all* $q \in [1,\infty)$;

(d) If $m_0 \in (0,1)$ *and in addition* f_0 *is continuous at* m_0, *then* $\sup_{x\in[0,1]} |(\tilde{g}_n - f_0)(x)| \xrightarrow{p} 0$.

Proposition 3.1.2 follows from Proposition 3.5.16 in Section 3.5.4, which handles the more general case where f_0 need not belong to $\mathcal{F}$, and where it may have multiple inflection points.

3.2 Computation of S-shaped least squares estimators

Returning to the setting of data $(x_1, Y_1), \ldots, (x_n, Y_n) \in [0,1] \times \mathbb{R}$ with $x_1 < \cdots < x_n$, we now consider the problem of computing an S-shaped LSE over $\mathcal{F}$. In light of the non-uniqueness discussion in Section 3.1, we will take as our target the LSE $\hat{f}_n := \hat{f}_n^{\hat{m}_n}$, where $\hat{m}_n := x_{\hat{\jmath}_n}$ and $\hat{\jmath}_n := \operatorname{sargmin}_{1\leq j\leq n} S_n(\hat{f}_n^{x_j})$; here and below, sargmin denotes the smallest element of the argmin. One of the main challenges here is that in general the function $j \mapsto S_n(\hat{f}_n^{x_j})$ has multiple local minima; see Figure 3.4. A 'brute-force' method that we call `ScanAll`, then, is to compute each of the LSEs $\hat{f}_n^{x_1}, \ldots, \hat{f}_n^{x_n}$ directly by solving n separate constrained least squares problems. In each instance, we can run the support reduction algorithm (Groeneboom et al., 2008) or a generic active set algorithm (Dümbgen et al., 2007; Nocedal and Wright, 2006, Chapters 12 and 16.5) on the whole

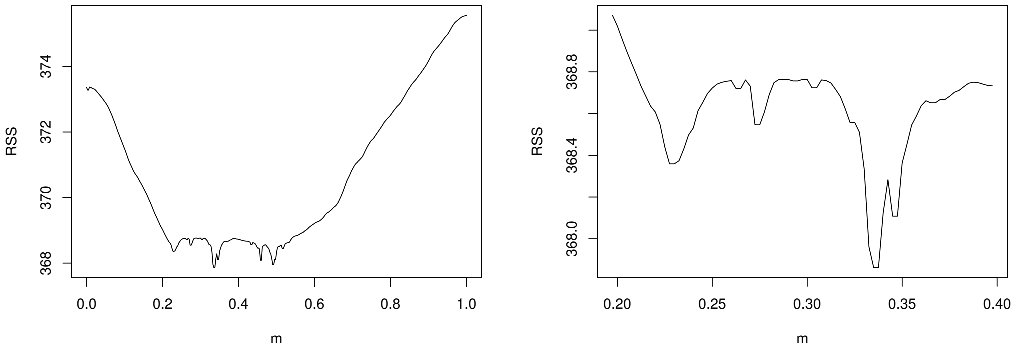

Figure 3.4: Plots of the residual sum of squares $S_n(\hat{f}_n^m)$ of the least squares estimator with inflection point at m over $m \in [0,1]$ (left) and $m \in [0.2, 0.4]$ (right), illustrating the multiple local minima of this function. Here, with $n = 400$, the data were generated according to $Y_i = f(x_i) + \xi_i$ for $i = 1, \dots, n$, with f taken to be the blue regression function from Figure 3.1, $x_i = i/n$ for $i = 1, \dots, n$ and $\xi_1, \dots, \xi_n$ independent $N(0,1)$ random errors.

dataset $\{(x_i, Y_i) : 1 \le i \le n\}$, but it is computationally expensive to repeat this n times, even when n is only moderately large; see Section 3.4.1. To improve the overall efficiency of this procedure, it would therefore be desirable to both refine the initial search strategy as well as exploit any common structure underlying the individual minimisation problems. For instance, we might hope to be able to obtain $\hat{f}_n^{x_j}$ via a faster update step that takes as input the previous LSE $\hat{f}_n^{x_{j-1}}$, but it is not immediately clear how this can be done.

We now describe and justify an alternative approach that achieves both of the above objectives. Our starting point is the following proposition, which reveals that the piecewise affine LSE $\tilde{f}_n$ can be 'decoupled' into left and right pieces, on which $\tilde{f}_n$ agrees with the increasing convex and increasing concave LSEs respectively. Let $\mathcal{H} \equiv \mathcal{H}[x_1, \dots, x_n] := \mathcal{F} \cap \mathcal{G}$ denote the set of S-shaped functions in $\mathcal{G}$, so that every $f \in \mathcal{F}$ agrees with some $h \in \mathcal{H}$ on $\{x_1, \dots, x_n\}$.

Proposition 3.2.1. *Let $\tilde{f}_n$ be any LSE over $\mathcal{H}$, and let $\tilde{m}_- = x_{\tilde{\jmath}_-}$ and $\tilde{m}_+ = x_{\tilde{\jmath}_+}$ be the smallest and largest inflection points of $\tilde{f}_n$ respectively. Define the intervals $L_- := [x_1, \tilde{m}_-]$, $R_- := (\tilde{m}_-, x_n]$, $L_+ := [x_1, \tilde{m}_+)$, $R_+ := [\tilde{m}_+, x_n]$ and $M := (\tilde{m}_-, \tilde{m}_+)$. Then for $A \in \{-, +\}$, the increasing convex LSE based on $\{(x_i, Y_i) : x_i \in L_A\}$ agrees with $\tilde{f}_n$ on L_A, and the increasing concave LSE based on $\{(x_i, Y_i) : x_i \in R_A\}$ agrees with $\tilde{f}_n$ on R_A. Moreover, the ordinary (linear) LSE, the increasing concave LSE and the increasing convex LSE based on $\{(x_i, Y_i) : x_i \in M\}$ all agree with $\tilde{f}_n$ on M.*

We explain in the third example following Proposition 3.5.4 that Proposition 3.2.1 is a consequence of Proposition 3.5.4(c, d, e), which also reveals that the result above is not guaranteed to hold if $\tilde{f}_n$ is replaced with $\hat{f}_n^m \in \mathcal{F}^m$ for a pre-specified $m \in \{x_1, \dots, x_n\}$. A further observation is that the localisation property in Proposition 3.2.1 is only valid for particular choices of partition of our data into subintervals, namely where the split occurs at the smallest or largest inflection points of $\tilde{f}_n$. In other words, for example, if we were to choose j such that $x_j < \tilde{m}_-$, then it would not in general be true that the LSE $\tilde{f}_n$ over $\mathcal{H}$ would agree on $[x_1, x_j]$ with the increasing convex LSE based on $\{(x_i, Y_i) : 1 \le i \le j\}$. This presents a substantial additional difficulty for both computation and theory in comparison with the problem of unimodal regression (Shoung and Zhang, 2001; Stout, 2008), where, for every jump x_j of the unimodal LSE $\tilde{g}_n$ to the left of its mode, it is the case that $\tilde{g}_n$ agrees on $[x_1, x_j]$ with the increasing LSE based on $\{(x_i, Y_i) : 1 \le i \le j\}$. These issues are discussed in greater depth in Section 3.5.1.

For $j \in [n]$,[†] we write $\hat{f}_{1,j} \in \mathcal{G}[x_1, \ldots, x_j]$ for the increasing convex LSE based on $\{(x_i, Y_i) : 1 \leq i \leq j\}$ and $\hat{f}_{n,j} \in \mathcal{G}[x_j, \ldots, x_n]$ for the increasing concave LSE based on $\{(x_i, Y_i) : j \leq i \leq n\}$. Since $\hat{f}_{1,j}(x_j) \geq Y_j$ and $\hat{f}_{n,j}(x_j) \leq Y_j$ for every $j \in [n]$ (e.g. Ghosal and Sen, 2017, Lemma 2.2), a direct consequence of Proposition 3.2.1 is the following:

Corollary 3.2.2. *In the setting of Proposition 3.2.1, we have* $Y_{\tilde{\jmath}_-} \leq \tilde{f}_n(x_{\tilde{\jmath}_-}) \leq \tilde{f}_n(x_{\tilde{\jmath}_-+1}) \leq Y_{\tilde{\jmath}_-+1}$ *and* $Y_{\tilde{\jmath}_+-1} \leq \tilde{f}_n(x_{\tilde{\jmath}_+-1}) \leq \tilde{f}_n(x_{\tilde{\jmath}_+}) \leq Y_{\tilde{\jmath}_+}$.

These two facts motivate the following generic procedure as an improvement on `ScanAll`:

Algorithm 1. Generic algorithm for computing $(\hat{m}_n, \hat{f}_n)$.

(I) Discard all $j \in [n]$ for which $Y_j > Y_{j+1}$.

(II) For each of the remaining indices j, compute $\hat{f}_{1,j}$ based on $\{(x_i, Y_i) : 1 \leq i \leq j\}$ and $\hat{f}_{n,j+1}$ based on $\{(x_i, Y_i) : j+1 \leq i \leq n\}$. Splicing these together, we define $\hat{h}_n^j \in \mathcal{G}[x_1, \ldots, x_n]$ by setting $\hat{h}_n^j(x_i) = \hat{f}_{1,j}(x_i)$ for $1 \leq i \leq j$ and $\hat{h}_n^j(x_i) = \hat{f}_{n,j+1}(x_i)$ for $j+1 \leq i \leq n$. Discard j if $\hat{h}_n^j \notin \mathcal{H}^{x_j}$, i.e. if

$$\frac{\hat{f}_{n,j+1}(x_{j+2}) - \hat{f}_{n,j+1}(x_{j+1})}{x_{j+2} - x_{j+1}} > \frac{\hat{f}_{n,j+1}(x_{j+1}) - \hat{f}_{1,j}(x_j)}{x_{j+1} - x_j}.$$

(III) Let $\mathcal{J}$ be the set of indices j that were not discarded in Steps 1 and 2. Find the smallest minimiser $\tilde{\jmath}$ of $j \mapsto s_n(j) := n^{-1} \sum_{i=1}^n \bigl(Y_i - \hat{h}_n^j(x_i)\bigr)^2$ over $\mathcal{J}$, and return $(x_{\tilde{\jmath}}, \hat{h}_n^{\tilde{\jmath}})$.

To see that the output $(x_{\tilde{\jmath}}, \hat{h}_n^{\tilde{\jmath}})$ of Algorithm 1 is indeed $(\hat{m}_n, \hat{f}_n)$, note first that since $\hat{m}_n = x_{\hat{\jmath}_n}$ is the smallest inflection point of the LSE $\hat{f}_n$ over $\mathcal{H}$, Corollary 3.2.2 ensures that $\hat{\jmath}_n$ is retained after Step I. For each index j in Step II, $\hat{h}_n^j$ is the minimiser of $f \mapsto S_n(f)$ over a subclass of $\mathcal{G}$ that contains $\mathcal{H}^{x_j}$, so if $\hat{h}_n^j \in \mathcal{H}^{x_j}$, then in fact $\hat{h}_n^j = \hat{f}_n^{x_j}$. In particular, this holds for $j = \hat{\jmath}_n$ by Proposition 3.2.1. Therefore, in Step III, $\hat{\jmath}_n \in \mathcal{J}$ and $s_n(j) = S_n(\hat{f}_n^{x_j})$ for all $j \in \mathcal{J}$, so $\tilde{\jmath} = \operatorname{sargmin}_{1 \leq j \leq n} S_n(\hat{f}_n^{x_j}) = \hat{\jmath}_n$. Thus, $x_{\tilde{\jmath}} = x_{\hat{\jmath}_n} = \hat{m}_n$ and $\hat{h}_n^{\tilde{\jmath}} = \hat{f}_n^{\hat{m}_n} = \hat{f}_n$, as desired.

The most obvious implementation of Step II of Algorithm 1 simply computes $\hat{f}_{1,j}$ and $\hat{f}_{n,j+1}$ from scratch for each different j; we refer to this as the `ScanSelected` algorithm. Even this naive modification has two significant advantages over `ScanAll`:

(i) In advance of carrying out any least squares minimisation, we can restrict the set of candidates for $\hat{\jmath}_n$ based on just $n-1$ pairwise comparisons. If $(x_1, Y_1), \ldots, (x_n, Y_n)$ are drawn according to a regression model (3.1.1) featuring a continuous f_0 and independent and identically distributed errors with zero mean, then Step I typically screens out about half of the indices in $[n]$ when n is reasonably large.

(ii) For the remaining indices j in Step II, we do not attempt to compute the S-shaped function $\hat{f}_n^{x_j}$ based on all n data points, but instead fit the increasing convex LSE $\hat{f}_{1,j}$ and the increasing concave LSE $\hat{f}_{n,j+1}$ using j and $n-j$ observations respectively.

The main drawback of the `ScanSelected` algorithm, however, is that it fails to exploit the commonalities in the computation of $\hat{f}_{1,j}$ for different j (and similarly of $\hat{f}_{n,j+1}$ for different j). Our main computational contribution, then, is to show that for $k \in [j-1]$, it is possible to obtain $\hat{f}_{1,j}$ by modifying $\hat{f}_{1,k}$ appropriately when the observations $\{(x_i, Y_i) : k < i \leq j\}$ are introduced. We can therefore proceed in a sequential manner and hence make significant computational gains.

[†]Here and below, we write $[n] := \{1, \ldots, n\}$ for $n \in \mathbb{N}$.

Recall that for $j \in [n]$ and a closed, convex cone $\Lambda \subseteq \mathbb{R}^j$, there exists a unique L^2-projection $\Pi_\Lambda \colon \mathbb{R}^j \to \Lambda$, given by

$$\Pi_\Lambda(y) := \operatorname*{argmin}_{u \in \Lambda} \|u - y\|.$$

The key to our approach is to develop a mixed primal-dual bases algorithm (Fraser and Massam, 1989; Meyer, 1999) that allows us to compute $\Pi_\Lambda(L)$ when $L \subseteq \mathbb{R}^j$ is a line segment and Λ is a polyhedral convex cone. An important observation is that, given $v(0), v(1) \in \mathbb{R}^j$, the map $t \mapsto \Pi_\Lambda\bigl((1-t)v(0) + tv(1)\bigr)$ is continuous and piecewise linear on $[0,1]$, where the individual linear pieces correspond to projections onto different faces of Λ; see Remark 3.5.1. This enables us to compute $\Pi_\Lambda\bigl(v(1)\bigr)$ when $\Pi_\Lambda\bigl(v(0)\bigr)$ is known. Indeed, we give a detailed description of a general procedure for this task in Section 3.5.2, and we focus here on its application to increasing convex regression (increasing concave regression for the right-hand end can be handled very similarly). In this case, the cones of particular interest to us are those of increasing convex sequences based on $x_1, \ldots, x_j$ for some $j \in [n]$, which we denote by

$$\Lambda^j := \bigl\{\bigl(g(x_1), \ldots, g(x_j)\bigr) : g \in \mathcal{F}^1\bigr\} = \left\{(z_1, \ldots, z_j) \in \mathbb{R}^j : 0 \le \frac{z_2 - z_1}{x_2 - x_1} \le \cdots \le \frac{z_j - z_{j-1}}{x_j - x_{j-1}}\right\}. \tag{3.2.1}$$

Given $k \in [j-1]$ and supposing that $\hat{f}_{1,k}$ has already been fitted, an appropriate choice of $v(0), v(1)$ is

$$v(0) = \bigl(Y_1, \ldots, Y_k, \hat{f}_{1,k}(x_{k+1}), \ldots, \hat{f}_{1,k}(x_j)\bigr) \quad \text{and} \quad v(1) = (Y_1, \ldots, Y_j), \tag{3.2.2}$$

because $\Pi_{\Lambda^j}\bigl(v(1)\bigr) = \bigl(\hat{f}_{1,j}(x_1), \ldots, \hat{f}_{1,j}(x_j)\bigr)$ is what we seek to compute, and moreover we claim that $\Pi_{\Lambda^j}\bigl(v(0)\bigr) = \bigl(\hat{f}_{1,k}(x_1), \ldots, \hat{f}_{1,k}(x_j)\bigr)$ (which is known). To establish this claim, observe that for any $u \equiv (u_1, \ldots, u_j) \in \Lambda^j$, we have

$$\|v(0) - u\|^2 \ge \sum_{i=1}^k (Y_i - u_i)^2 \ge \sum_{i=1}^k \bigl(Y_i - \hat{f}_{1,k}(x_i)\bigr)^2 = \bigl\|v(0) - \bigl(\hat{f}_{1,k}(x_1), \ldots, \hat{f}_{1,k}(x_j)\bigr)\bigr\|^2, \tag{3.2.3}$$

and $\bigl(\hat{f}_{1,k}(x_1), \ldots, \hat{f}_{1,k}(x_j)\bigr) \in \Lambda^j$. In fact, we will apply this version of the mixed primal-dual bases algorithm with $k = j-1$, so that the observations $Y_1, \ldots, Y_n$ are introduced sequentially. Note that when $Y_j \ge \hat{f}_{1,j-1}(x_j)$, we have by the same argument as in (3.2.3) that $\bigl(\hat{f}_{1,j}(x_1), \ldots, \hat{f}_{1,j}(x_j)\bigr) = \bigl(\hat{f}_{1,j-1}(x_1), \ldots, \hat{f}_{1,j-1}(x_{j-1}), Y_j\bigr)$, so no calculations are required. We refer to our implementation of this algorithm as `SeqConReg`.

3.3 Theoretical properties of S-shaped least squares estimators

3.3.1 Worst-case and adaptive sharp oracle inequalities

Our first main results of this section consist of worst-case and adaptive sharp oracle inequalities for S-shaped least squares estimators. These reveal not only risk bounds when our S-shaped regression function hypothesis is correctly specified, but also control the way in which the performance of the estimators deteriorate as the model becomes increasingly misspecified.

We will work in the setting of model (3.1.1), but now make the following assumption on the errors:

Assumption 1. *$\{\xi_i \equiv \xi_{ni} : 1 \le i \le n\}$ is a collection of independent sub-Gaussian random variables with parameter 1, so that $\mathbb{E}(e^{t\xi_{ni}}) \le e^{t^2/2}$ for all $t \in \mathbb{R}$ and $i \in [n]$.*

For fixed $n \in \mathbb{N}$ and $f\colon [0,1] \to \mathbb{R}$, we write $x_i \equiv x_{ni}$ for $i \in [n]$ and let $\|f\|_n := \|f\|_{L^2(\mathbb{P}_n^X)} = \bigl(\sum_{i=1}^n f^2(x_i)/n\bigr)^{1/2}$. Also, for $f \in \mathcal{H} \equiv \mathcal{H}[x_1, \dots, x_n]$, let $V(f) := f(x_n) - f(x_1) = \max_{1 \le i \le n} f(x_i) - \min_{1 \le i \le n} f(x_i)$ and denote by $k(f)$ the number of affine pieces of f, so that $k(f)$ is the smallest $k \in [n]$ with the property that f is affine on each of k subintervals $I_1, \dots, I_k$ that partition $[0,1]$.

Theorem 3.3.1. *For fixed $n \ge 2$, suppose that Assumption 1 holds and let $\tilde{f}_n$ be any LSE over $\mathcal{F}$. Let $R := n^{-1}(x_n - x_1)/\min_{2 \le i \le n}(x_i - x_{i-1})$. Then there exists a universal constant $C > 0$ such that for every $f_0\colon [0,1] \to \mathbb{R}$ and $t > 0$, we have*

$$\|\tilde{f}_n - f_0\|_n \le \inf_{f \in \mathcal{H}} \biggl\{ \|f - f_0\|_n + \frac{C\bigl(1 + V(f)\bigr)^{1/3}}{n^{1/3}} \wedge \frac{CR^{1/10}\bigl(1 + V(f)\bigr)^{1/5}}{n^{2/5}} \biggr\} + \sqrt{\frac{8t}{n}} \tag{3.3.1}$$

with probability at least $1 - e^{-t}$.

By integrating this tail bound, we obtain the worst-case risk bound

$$\mathbb{E}_{f_0}(\|\tilde{f}_n - f_0\|_n) \le \inf_{f \in \mathcal{H}} \biggl\{ \|f - f_0\|_n + \frac{C\bigl(1 + V(f)\bigr)^{1/3}}{n^{1/3}} \wedge \frac{CR^{1/10}\bigl(1 + V(f)\bigr)^{1/5}}{n^{2/5}} \biggr\} + \sqrt{\frac{2\pi}{n}}. \tag{3.3.2}$$

In the special case where $f_0 \in \mathcal{F}$, we may take $f = f_0$ in Theorem 3.3.1 to conclude that[‡]

$$\mathbb{E}_{f_0}(\|\tilde{f}_n - f_0\|_n) \lesssim \frac{\bigl(1 + V(f_0)\bigr)^{1/3}}{n^{1/3}} \wedge \frac{R^{1/10}\bigl(1 + V(f_0)\bigr)^{1/5}}{n^{2/5}};$$

thus, when R and $V(f_0)$ are of constant order, we obtain a worst-case risk bound of order $n^{-2/5}$. More generally, (3.3.1) and (3.3.2) reveal the impact of both non-equispaced design and the range of the signal. In fact, an alternative, more complicated definition of R is possible, and this further refines our bounds for certain designs; see the discussion following the proof of Theorem 3.3.1 in Section 3.5.3. To see that the rate of order $n^{-2/5}$ cannot in general be attained for arbitrary configurations of design points, we appeal to Bellec (2018, Theorem 4.5) for a suitable minimax lower bound: for any $V \ge n^{-1/2}$, there exist design points $x_1 < \cdots < x_n$ that depend on V such that if $\xi_1, \dots, \xi_n \overset{\text{iid}}{\sim} N(0,1)$ in (3.1.1), then

$$\inf_{\breve{g}_n} \sup_{f_0 \in \mathcal{F}^1 : V(f_0) \le 2V} \mathbb{P}_{f_0}\bigl(\|\breve{g}_n - f_0\|_n \ge C(V/n)^{1/3}\bigr) \ge c,$$

where the infimum is taken over all estimators $\breve{g}_n \equiv \breve{g}_n(x_1, Y_1, \dots, x_n, Y_n)$, and $c, C > 0$ are universal constants.

Another very attractive aspect of Theorem 3.3.1 is that, in cases where $f_0 \notin \mathcal{F}$, we can control the performance of an LSE $\tilde{f}_n$ over $\mathcal{F}$ via approximation error and estimation error terms. The fact that the approximation error term $\|f - f_0\|_n$ has leading constant 1 (which is the best possible) is the reason that (3.3.1) and (3.3.2) are referred to as sharp oracle inequalities.

To complement the worst-case sharp oracle inequality in (3.3.2), we now consider the more favourable situation where f_0 is well approximated by a piecewise affine function with not too many affine pieces. The fact that an LSE $\tilde{f}_n$ over $\mathcal{F}$ can approximate such a signal with a relatively small number of kinks suggests that we may be able to obtain improved sharp oracle inqualities in such cases.

[‡]Here and below, we write $a_n \lesssim b_n$ to mean that there exists a universal constant $C > 0$ such that $a_n \le Cb_n$ for all n.

Theorem 3.3.2. *For fixed $n \geq 2$, suppose that Assumption 1 holds, and let $\tilde{f}_n$ be any LSE over $\mathcal{F}$. Then for every $f_0 \colon [0,1] \to \mathbb{R}$ and $t > 0$, we have*

$$\|\tilde{f}_n - f_0\|_n \leq \inf_{f \in \mathcal{H}} \left\{ \|f - f_0\|_n + \sqrt{\frac{32\bigl(k(f)+1\bigr)}{n} \log\left(\frac{en}{k(f)+1}\right)} \right\} + \sqrt{\frac{2(t + \log n)}{n}} \tag{3.3.3}$$

with probability at least $1 - e^{-t}$.

As with Theorem 3.3.1, we can integrate the tail bound from (3.3.3) to obtain

$$\begin{aligned} \mathbb{E}_{f_0}(\|\tilde{f}_n - f_0\|_n) &\leq \inf_{f \in \mathcal{H}} \left\{ \|f - f_0\|_n + \sqrt{\frac{32\bigl(k(f)+1\bigr)}{n} \log\left(\frac{en}{k(f)+1}\right)} \right\} + \sqrt{\frac{2 \log n}{n}} + \sqrt{\frac{\pi}{2n}} \\ &\leq \inf_{f \in \mathcal{H}} \left\{ \|f - f_0\|_n + 8\sqrt{\frac{k(f)+1}{n} \log\left(\frac{en}{k(f)+1}\right)} \right\}. \end{aligned} \tag{3.3.4}$$

In particular, we see from (3.3.4) that if $f_0 \in \mathcal{F}$ has k affine pieces, then any LSE $\tilde{f}_n$ over $\mathcal{F}$ attains the parametric rate $k^{1/2}/n^{1/2}$, up to a logarithmic factor.

3.3.2 Inflection point estimation

A particular feature of estimating S-shaped functions that differentiates it from other shape-constrained estimation problems is the existence of an inflection point m_0. In some respects, this is like a boundary point, because it represents the point of transition from convex to concave parts of the function, and the behaviour of the function is therefore less regulated there (in particular, the derivative of an S-shaped function may diverge to infinity as we approach the inflection point). On the other hand, when $m_0 \in (0,1)$, we may well have design points on either side of m_0, and in that sense the inflection point may be regarded as an interior point. The distinguished nature of the inflection point means that its location is often of interest in applications such as economic growth modelling (e.g. Jarne et al., 2007).

In studying the inflection point estimation problem, we will assume that $f_0 \in \mathcal{F}$ and the following additional conditions hold:

Assumption 2. *Suppose that $f_0 \in \mathcal{F}$ has a unique inflection point $m_0 \in (0,1)$, and that there exist $B > 0$ and $\alpha \in (0,1) \cup (1,\infty)$ such that as $x \to m_0$, we have*

$$f_0(x) = \begin{cases} f_0(m_0) - B\bigl(1 + o(1)\bigr)\operatorname{sgn}(x - m_0)|x - m_0|^\alpha & \text{when } \alpha \in (0,1) \\ f_0(m_0) + f_0'(m_0)(x - m_0) + B\bigl(1 + o(1)\bigr)\operatorname{sgn}(x - m_0)|x - m_0|^\alpha & \text{when } \alpha > 1. \end{cases} \tag{3.3.5}$$

In the regression model (3.1.1), suppose also that $x_{ni} = i/n$ and $\xi_{ni} \overset{d}{=} \xi$ for all $n \in \mathbb{N}$ and $i \in [n]$, where ξ is a sub-Gaussian random variable with parameter 1.

When $\alpha \geq 3$ is an integer, (3.3.5) holds if (a) f_0 is α-times continuously differentiable in a neighbourhood of m_0, and (b) $f_0^{(k)}(m_0) = 0 \neq f_0^{(\alpha)}(m_0)$ for $2 \leq k \leq \alpha - 1$. Under this stronger assumption, α must in fact be odd, and $f_0^{(\alpha)}(m_0) < 0$. Indeed, for all $x \in [0,1]$ sufficiently close to the inflection point m_0, we have $f_0''(x) \geq 0$ if $x \leq m_0$ and $f_0''(x) \leq 0$ if $x \geq m_0$, and since $f_0^{(\alpha)}$ is continuous at m_0, a Taylor expansion reveals that $f_0''(x) = f_0^{(\alpha)}(m_0)\bigl(1 + o(1)\bigr)(x - m_0)^{\alpha-2}/(\alpha-2)!$ as $x \to m_0$.

Theorem 3.3.3. *Let $(\tilde{f}_n)$ be any sequence of LSEs over $\mathcal{F}$, and for each n, let $\tilde{m}_n$ be an inflection point of $\tilde{f}_n$. Under Assumption 2, we have $\tilde{m}_n - m_0 = O_p\bigl((n/\log n)^{-1/(2\alpha+1)}\bigr)$.*

We mention that Liao and Meyer (2017) study a least squares estimator over a subclass of $\mathcal{F}$ consisting of cubic splines (where the number of knots is of order $n^{1/9}$); they show that its inflection point converges to the true m_0 at rate $O_p(n^{-8/63})$ in a random design setting where f_0 satisfies (a stronger version of) (3.3.5) with $\alpha = 3$. The proof of their Theorem 2 relies on a quantitative result on the quality of local approximations to f_0 near m_0 by convex or concave functions (Liao and Meyer, 2017, Lemma 2), as well as a global rate of convergence for their spline-based estimator.

In our setting, Theorem 3.3.3 shows that the inflection point estimator $\tilde{m}_n$ (based on an LSE $\tilde{f}_n$ over the entire class $\mathcal{F}$) converges to m_0 at rate $O_p\big((n/\log n)^{-1/7}\big)$ when $\alpha = 3$. The proof of Theorem 3.3.3, which is given in Section 3.5.3, is lengthy and broken up into several steps, each of which requires some delicate technical arguments; see Figure 3.9 for an illustration. The crucial Step 2a exploits the observation that if $\tilde{m}_n$ is a long way from m_0, then there is a long interval between the two on which one of $f_0, \tilde{f}_n$ is convex and the other is concave. On such an interval, we show that $\tilde{f}_n$ has a long affine piece, as would be intuitively expected, and thereby quantify the approximation error due to misspecification; see Lemma 3.5.9. Another important aspect of our proof strategy is that we find a suitable way to localise the analysis of $\tilde{f}_n$ to a neighbourhood of m_0, rather than rely on global considerations that would lead to a suboptimal bound. As we explain in Section 3.5.1, our localisation technique for convex or S-shaped LSEs relies on non-trivial 'boundary adjustments' that are not needed for isotonic or unimodal LSEs. Nevertheless, a simpler version of the proof of Theorem 3.3.3 allows us to recover the result of Shoung and Zhang (2001) on the rate of convergence of the mode of the LSE of a unimodal regression function, at least under our sub-Gaussian assumption on the errors ξ_{ni} and their local smoothness condition (1.3).

The rate of convergence of $\tilde{m}_n$ to m_0 in Theorem 3.3.3 matches that in the following complementary local asymptotic minimax lower bound, up to a logarithmic factor. For $r > 0$, let $\mathcal{F}(f_0, r) := \{f \in \mathcal{F} : \int_0^1 (f - f_0)^2 < r^2\}$. Although f_0 has a unique inflection point m_0 under Assumption 2, not every function in $\mathcal{F}(f_0, r)$ has a unique inflection point, so for $f \in \mathcal{F}$, we denote by $\mathcal{I}_f$ the subinterval of inflection points of f and define $d(x, \mathcal{I}_f) := \inf_{z \in \mathcal{I}_f} |x - z|$ for $x \in [0, 1]$.

Proposition 3.3.4. *Under Assumption 2, and with $\xi_{n1}, \ldots, \xi_{nn} \overset{\text{iid}}{\sim} N(0,1)$ for all n, we have*

$$\sup_{\tau > 0} \liminf_{n \to \infty} \inf_{\check{m}_n} \sup_{f \in \mathcal{F}(f_0, \tau/\sqrt{n})} n^{1/(2\alpha+1)}\, \mathbb{E}_f\big(d(\check{m}_n, \mathcal{I}_f)\big) > 0, \tag{3.3.6}$$

where the infimum is taken over all estimators $\check{m}_n \equiv \check{m}_n(x_1, Y_1, \ldots, x_n, Y_n)$ taking values in $[0, 1]$, and $\mathbb{E}_f$ is the expectation operator under the model (3.1.1) with f in place of f_0.

3.4 Simulations

In this section, we investigate the computation time and the empirical performance of our S-shaped estimator in some numerical experiments.

3.4.1 Computation time

We compare the running time of our sequential cone projection Algorithm 2, denoted as `SeqConReg`, with two other possible approaches. The first, which we call `ScanAll`, relies on a brute-force search that scans through all possible inflection points $m \in \{x_1, \ldots, x_n\}$ as described in the introduction, performing least squares over $\mathcal{F}^m$, and determining the candidate that minimises the residual sum of squares. Here the active set least squares procedure used for each m is based on a simple modification of the `R` package `scar` (Chen and Samworth, 2014, 2016). The second approach, which we call `ScanSelected`, is based on the observation in Step I of Algorithm 1 that there is no need to scan through all design points. Instead, we restrict attention to those indices j for which $Y_j \leq Y_{j+1}$, fitting a convex increasing function to $\{(x_i, Y_i) : 1 \leq i \leq j\}$, a concave and increasing function to $\{(x_i, Y_i) : j+1 \leq i \leq n\}$ (both using `scar`), before finding the smallest j that minimises the residual sum of squares.

For $n \in \{100, 200, 500, 1000\}$, we set $x_i = i/(n+1)$ and $Y_i = \sin(x_i - 0.5) + \sigma\epsilon_i$ for $i = 1, \ldots, n$, where $\epsilon_1, \ldots, \epsilon_n$ are independent normal random variables with zero mean and unit variance. Here, to examine the impact of the signal-to-noise ratio on the running time, we also vary the value of $\sigma \in \{1, 0.1, 0.01\}$, and plot the average running time of the different approaches in Figure 3.5. We see that `SeqConReg` is the fastest among all three approaches, being approximately 10 times more efficient than `ScanSelected` and 40 times faster than `ScanAll`. The ratio of the timings becomes larger as the signal-to-noise ratio increases, because the resulting fitted function has more knots, which makes it more appealing to use algorithms of a sequential nature, such as `SeqConReg`.

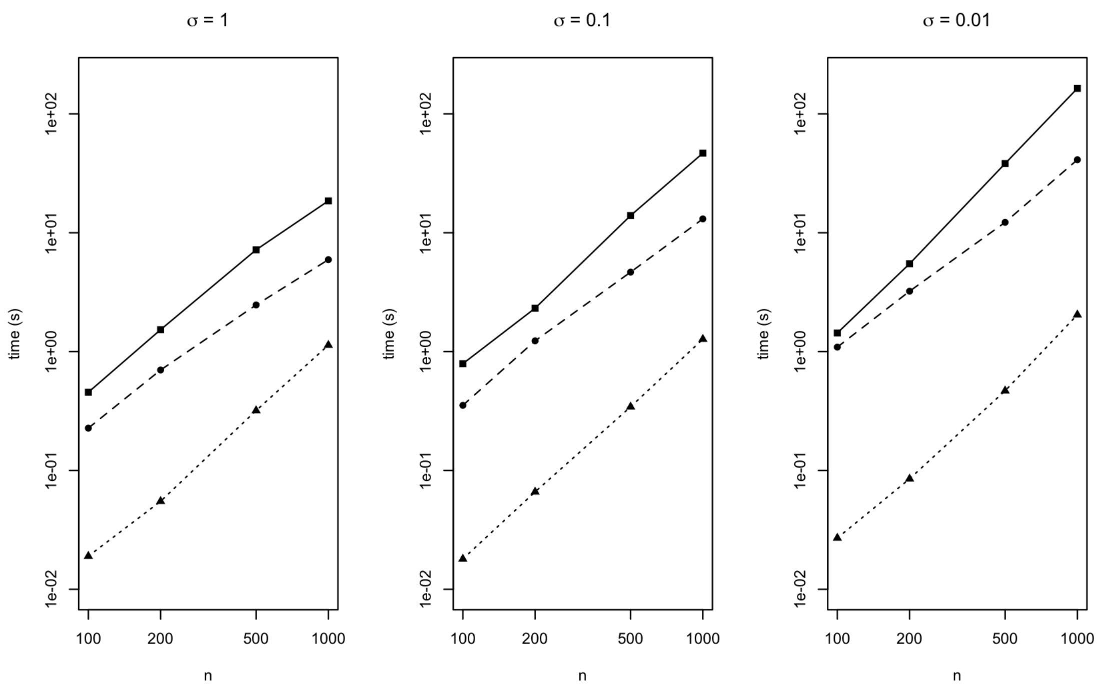

Figure 3.5: Log-log plots of the running time (in seconds) of the `SeqConReg` (▲), `ScanSelected` (●) and `ScanAll` (■) algorithms for least squares estimation of an S-shaped function, for sample sizes $n \in \{100, 200, 500, 1000\}$ and noise levels $\sigma \in \{1, 0.1, 0.01\}$.

3.4.2 Statistical performance

We compare our estimator (denoted as LSE) with the following alternatives: Liao and Meyer (2017) based on cubic B-splines with shape constraints, implemented in the `R` package `ShapeChange` (Liao and Meyer, 2016), and denoted as Spline; the shape-constrained kernel least squares method of Yagi et al. (2019, 2020) based on local linear kernels, denoted as SCKLS;[§] the bisection extremum distance estimator and bisection extremum surface estimator of Christopoulos (2016), both developed based on the geometric properties of the inflection point for a smooth function and implemented in the `R` package `inflection` (Christopoulos, 2019), which we denote as BEDE and BESE, respectively. For LSE, Spline and SCKLS, we assess their performance based on both the average $L^2(\mathbb{P}_n)$ loss and the mean absolute error of the estimated inflection point location, while for BEDE and BESE

[§]To give more implementation details, we run SCKLS with $M = 50$ evaluation points and select the kernel bandwidth according to the method of Ruppert, Sheather and Wand (1995).

we compute only the mean absolute error of the estimated inflection point location. All results are based on numerical experiments over 1000 repetitions.

For $n \in \{100, 200, 500, 1000\}$, and design points $x_1, \ldots, x_n$, we set $Y_i = f_j(x_i) + 0.1\epsilon_i$ for $i = 1, \ldots, n$, where $\epsilon_1, \ldots, \epsilon_n \overset{\text{iid}}{\sim} N(0,1)$, for four different choices of signal function f_j:

$$f_1(x) = \begin{cases} 2(0.3 - \sqrt{0.09 - x^2}) & \text{for } x \in [0, 0.3) \\ 2\{0.3 + \sqrt{0.49 - (1-x)^2}\} & \text{for } x \in [0.3, 1] \end{cases}; \qquad f_3(x) = x + \mathbb{1}_{\{x \geq 0.3\}};$$

$$f_2(x) = \sin\{(x - 0.3)\pi/1.4\}\mathbb{1}_{\{x \geq 0.3\}}; \qquad f_4(x) = 4/\{1 + e^{-2(x-0.3)}\}. \quad (3.4.1)$$

These signals are plotted in Figure 3.6. The signals are designed in such a way that their ranges over $[0, 1]$ are roughly the same. Furthermore, they all belong to $\mathcal{F}$ and have a unique inflection point at $m_0 = 0.3$. Note that f_1 satisfies Assumption 2 with $\alpha = 1/2$, and f_2 and f_3 do not satisfy Assumption 2 for any $\alpha > 0$, while f_4 satisfies the assumption with $\alpha = 3$.

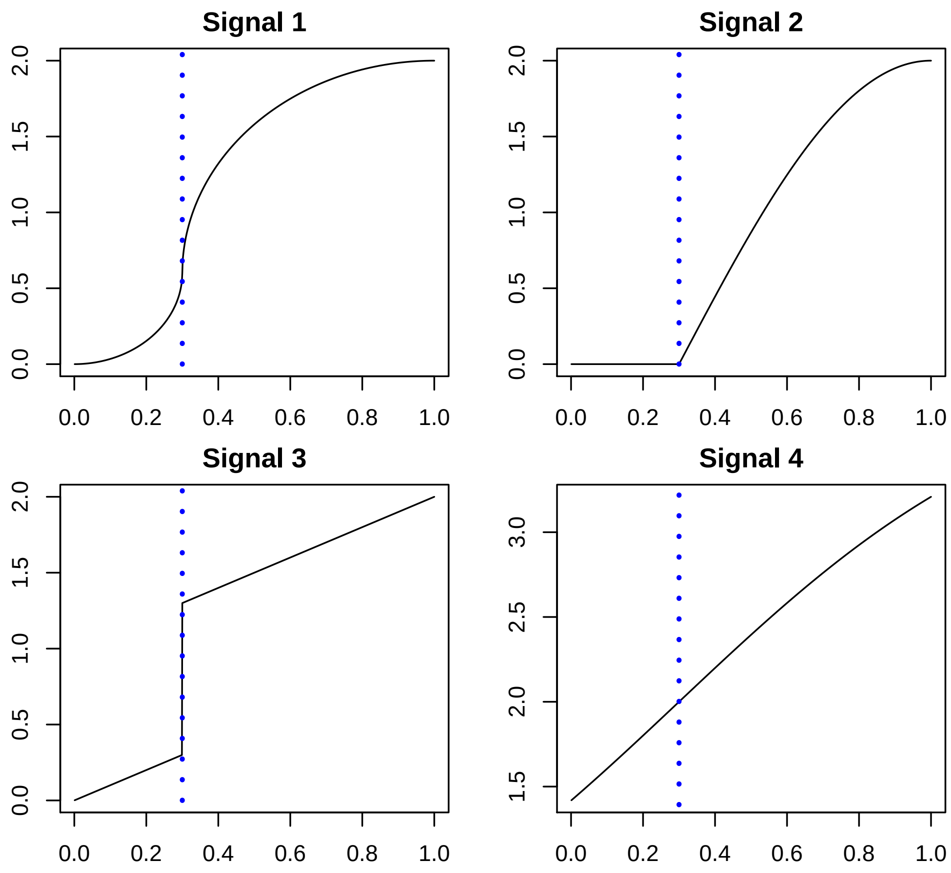

Figure 3.6: Plots of the signals f_1, f_2, f_3, f_4 defined in (3.4.1), with the inflection points highlighted by dashed blue lines.

We consider two different designs by setting $x_i = F^{-1}\big(i/(n+1)\big)$ for $i = 1, \ldots, n$, where F is the distribution function of either the $U[0, 1]$ or $\text{Beta}(4, 8)$ distribution. In the second setting, the design points are not equally spaced, and $m_0 = 0.3$ is the mode of the $\text{Beta}(4, 8)$ distribution. The results are shown in Figures 3.7 and 3.8.

For the estimation of the regression function, the LSE performs well in all cases; in particular, it is able to adapt to inhomogeneous smoothness levels and asymmetric designs. On the other hand, the spline- and kernel-based approaches struggle in this regard, and perform much worse for signals f_1 and f_3 especially. In fact, the spline-based method appears to be inconsistent for signals f_1 and f_3, and the kernel-based approach seems to suffer the same problem for signal f_3 too. For the estimation of the inflection point, the story has some similarities, but also some differences: for signals f_1, f_2 and f_3, the least squares approach provides more reliable estimates, for two main reasons. First, it is able to adapt to a much wider range of local smoothnesses around m_0. Second, by carefully comparing Figure 3.8 to Figure 3.7, we see that the least squares approach is also able to take advantage of the additional design points near m_0 under the beta design to obtain improved estimation performance (relative to the uniform design). For signal f_4, the other methods are able to exploit the homogeneity of the signal across the entire domain (and the symmetry of the signal around the inflection point) and tend to have smaller mean absolute error than the least squares approach. We recall Figure 3.2, which further illustrates the dangers of assuming smoothness of an S-shaped signal when it is not present.

3.5 Proofs of main results and computational details

3.5.1 Subinterval localisation and boundary adjustment results

As in Section 3.2, we consider pairs $(x_1, Y_1), \ldots, (x_n, Y_n)$ taking values in $[0,1] \times \mathbb{R}$, where $0 \leq x_1 < \cdots < x_n \leq 1$ are fixed. The purpose of this subsection is to generalise the following, known 'subinterval localisation' property of the univariate isotonic LSE $\bar{f}_n$ based on $\{(x_i, Y_i) : 1 \leq i \leq n\}$: if $\bar{f}_n$ has a jump after x_k, so that $\bar{f}_n(x_k) < \bar{f}_n(x_{k+1})$, then the isotonic LSE based on $\{(x_i, Y_i) : 1 \leq i \leq k\}$ agrees with $\bar{f}_n$ on $[x_1, x_k]$, and the isotonic LSE based on $\{(x_i, Y_i) : k+1 \leq i \leq n\}$ agrees with $\bar{f}_n$ on $[x_{k+1}, x_n]$. One way to see this is to invoke the explicit representation of $\bar{f}_n$ as the left derivative of the greatest convex minorant of the cumulative sum diagram associated with $(x_1, Y_1), \ldots, (x_n, Y_n)$ (e.g. Groeneboom and Jongbloed, 2014, Lemma 2.1).

By comparison with the isotonic LSE, the lack of an explicit representation makes the situation much more complicated for convex and concave LSEs, as well as the S-shaped LSEs (with known or unknown inflection point $m \in [0,1]$) defined in Section 3.1. Writing $\tilde{g}_n$ for any one of these LSEs and x_k for one of its kinks, we will see below that $\tilde{g}_n$ cannot in general be localised exactly to either $[x_1, x_k]$ or $[x_k, x_n]$. In fact, one of our significant technical contributions is to show that, on each of these subintervals, the restriction of $\tilde{g}_n$ minimises a *weighted* sum of squares, in which the observation (x_k, Y_k) is assigned a fraction of the weight placed on all the other points in the subinterval; see (3.5.1). Although the adjusted 'boundary weight' usually depends on the LSE $\tilde{g}_n$ and is not an accessible quantity in its own right, the merit of this boundary reweighting idea is seen in the proof of Theorem 3.3.3 on inflection point estimation. A special case where no boundary adjustment is needed (Proposition 3.2.1) is the basis of Algorithm 1 for computing S-shaped LSEs.

The subinterval localisation properties of all the LSEs mentioned above will be derived as consequences of the general Lemma 3.5.1 below, for which we require the following additional notation. Let $\mathbf{1} := (1, 1, \ldots, 1) = \sum_{i=1}^n e_i \in \mathbb{R}^n$, where $e_1, \ldots, e_n$ are the standard basis vectors in $\mathbb{R}^n$. For $1 \leq a \leq b \leq n$, let $\mathbf{1}^{[a:b]} := \sum_{i=a}^b e_i$, and for $\theta \in \mathbb{R}^n$, define $\theta^{(a:b)} \in \mathbb{R}^n$ by $\theta_i^{(a:b)} := \theta_{a \vee i \wedge b}$ for $i \in [n]$. In addition, for $w \equiv (w_1, \ldots, w_n) \in [0, \infty)^n$ and $u, v \in \mathbb{R}^n$, define $\langle u, v \rangle_w := \sum_{i=1}^n w_i u_i v_i$ and $\|u\|_w := \langle u, u \rangle_w^{1/2}$, so that $\langle \cdot, \cdot \rangle_w$ is a non-negative definite symmetric bilinear form. It is convenient to study weighted LSEs defined with respect to arbitrary weight vectors $w \in [0, \infty)^n$, even though we are primarily interested in the case $w = \mathbf{1}$ in subsequent applications of the result below.

Lemma 3.5.1. *Let $\Theta \subseteq \mathbb{R}^n$ be a closed, convex set, let $Y := (Y_1, \ldots, Y_n) \in \mathbb{R}^n$ and, for some weight vector $w \equiv (w_1, \ldots, w_n) \in [0, \infty)^n$, let $\hat{\theta} \equiv \hat{\theta}_n(w) \in \operatorname{argmin}_{\theta \in \Theta} \|Y - \theta\|_w$. Suppose that $\hat{\theta} \pm \eta \mathbf{1} \in \Theta$ for some $\eta > 0$.*

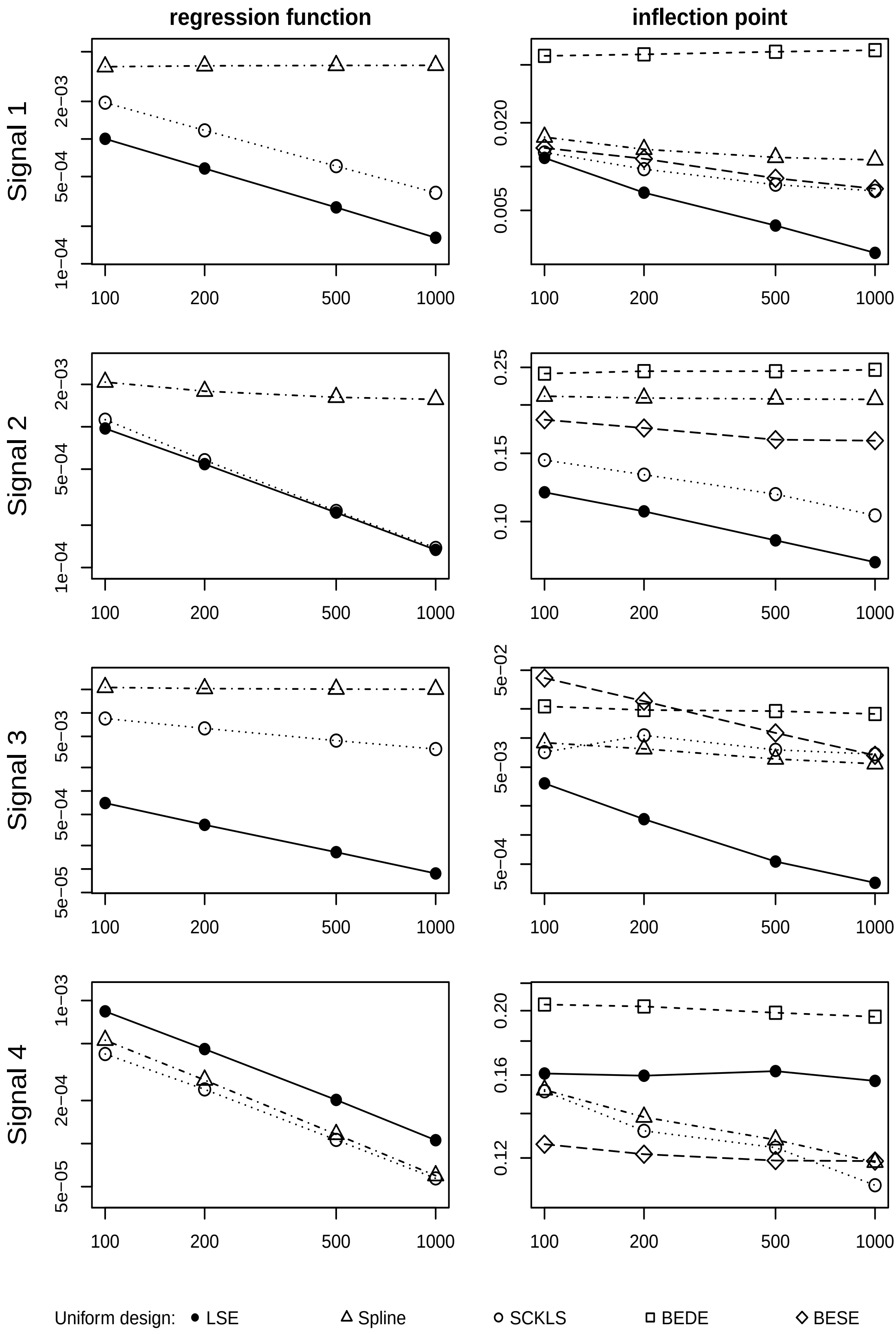

Figure 3.7: Log-log plots of the mean squared error of the fitted function on the design points, as well as the mean absolute distance between the estimated and true inflection points, based on $n = 100, 200, 500, 1000$ observations when the design points are equispaced and the signals are as in Figure 3.6.

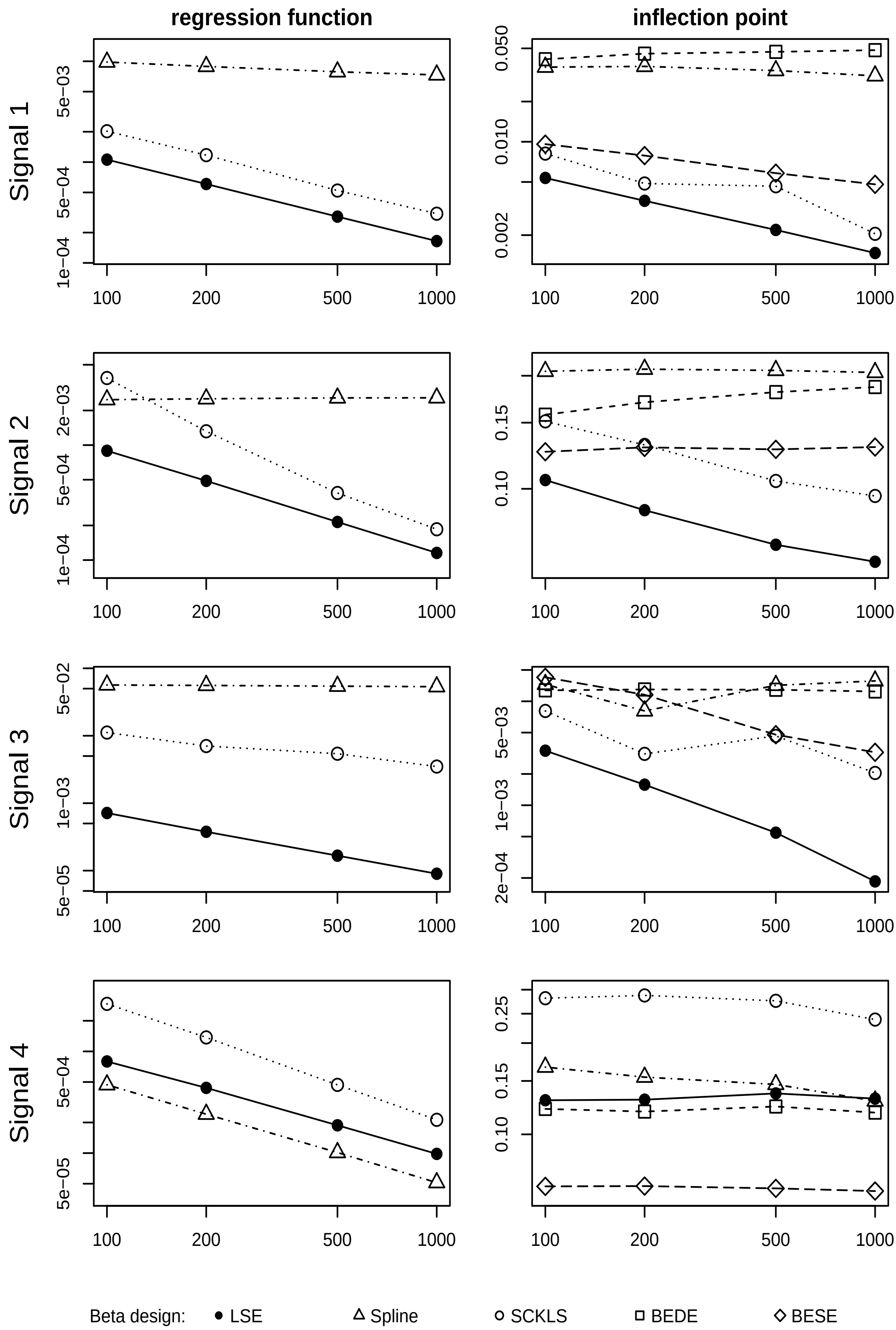

Figure 3.8: Log-log plots of the mean squared error of the fitted function on the design points, as well as the mean absolute distance between the estimated and true inflection points, based on $n = 100, 200, 500, 1000$ observations when the design points are quantiles of a Beta$(4, 8)$ distribution and the signals are as in Figure 3.6.

(a) *Assume that at least one of the following conditions is satisfied for some* $k \in [n]$*:*

(i) $\hat{\theta} + \varepsilon\eta\mathbf{1}^{[1:k]} \in \Theta$ *and* $\hat{\theta} + \varepsilon\eta\mathbf{1}^{[k:n]} \in \Theta$ *for some* $\varepsilon \in \{-1, 1\}$ *and* $\eta > 0$*;*

(ii) $\hat{\theta} \pm \eta u \in \Theta$ *for some* $u \in \{\mathbf{1}^{[1:k]}, \mathbf{1}^{[k:n]}\}$ *and* $\eta > 0$*.*

Then defining

$$\underline{w}_k := \frac{\sum_{i=1}^{k-1} w_i(Y_i - \hat{\theta}_i)}{\hat{\theta}_k - Y_k} \mathbb{1}_{\{\hat{\theta}_k \neq Y_k\}} \quad \text{and} \quad \overline{w}_k := \frac{\sum_{i=k+1}^{n} w_i(Y_i - \hat{\theta}_i)}{\hat{\theta}_k - Y_k} \mathbb{1}_{\{\hat{\theta}_k \neq Y_k\}}, \tag{3.5.1}$$

we have $\underline{w}_k, \overline{w}_k \in [0, w_k]$ *and* $\underline{w}_k + \overline{w}_k \leq w_k$*, with equality when* $Y_k \neq \hat{\theta}_k$*.*

If (ii) holds with $u = \mathbf{1}^{[1:k]}$*, then* $\overline{w}_k = 0$*, and if (ii) holds with* $u = \mathbf{1}^{[k:n]}$*, then* $\underline{w}_k = 0$*.*

(b) *Let* $1 \leq a \leq b \leq n$ *be such that for each* $k \in \{a, b\}$*, either (i) or (ii) holds, and suppose that for each* $\theta \in \Theta \cup \{-\hat{\theta}\}$*, there exists* $\eta > 0$ *such that* $\hat{\theta} + \eta\theta^{(a:b)} \in \Theta$*. Then defining*

$$\tilde{w}^{a;b} := (0, \ldots, 0, \overline{w}_a, w_{a+1} \ldots, w_{b-1}, \underline{w}_b, 0, \ldots, 0) \in \mathbb{R}^n, \tag{3.5.2}$$

so that $\tilde{w}_i^{a;b} = 0$ *for* $1 \leq i < a$ *and* $b < i \leq n$*, we have* $\hat{\theta} \in \operatorname{argmin}_{\theta \in \Theta} \|Y - \theta\|_{\tilde{w}^{a;b}}$*.*

The main conclusion of Lemma 3.5.1 comes at the end of part (b): under certain conditions on a, b, there exists a non-negative weight vector $\tilde{w}^{a;b}$, whose only non-zero weights occur for indices i with $a \leq i \leq b$, for which the sub-vector $(\hat{\theta}_a, \hat{\theta}_{a+1}, \ldots, \hat{\theta}_b)$ of the overall LSE $\hat{\theta}$ can be computed as the $\tilde{w}^{a;b}$-weighted LSE of our data vector Y. Note that $\tilde{w}^{a;b}$ differs from $w^{a;b}$ only at the endpoints a and b; we therefore refer to $\tilde{w}^{a;b}$ as the *boundary-adjusted weight vector*. Condition (ii) in (a) yields sufficient conditions for exact subinterval localisation (without non-trivial boundary adjustments $\underline{w}_k, \overline{w}_k$). Since it is assumed that $\hat{\theta} \pm \eta\mathbf{1} \in \Theta$ for some $\eta > 0$, condition (ii) in (a) holds for $k \in \{1, n\}$; although this is vacuous as far as the conclusion of (a) is concerned, it means that we can take $a = 1$ or $b = n$ in (b).

Proof. For a closed, convex set $\Theta \subseteq \mathbb{R}^n$ and a weight vector $w \in [0, \infty)^n$, the existence of $\hat{\theta} \in \operatorname{argmin}_{\theta \in \Theta} \|Y - \theta\|_w$ is guaranteed (and uniqueness holds if $w_i > 0$ for all $i \in [n]$). In all cases, we have $\hat{\theta} \in \operatorname{argmin}_{\theta \in \Theta} \|Y - \theta\|_w$ if and only if

$$\langle Y - \hat{\theta}, \theta - \hat{\theta} \rangle_w = \sum_{i=1}^{n} w_i(Y_i - \hat{\theta}_i)(\theta_i - \hat{\theta}_i) \leq 0 \tag{3.5.3}$$

for all $\theta \in \Theta$; see Lemma 3.6.1(a).

(a) By assumption, we can take $\theta = \hat{\theta} \pm \eta\mathbf{1} \in \Theta$ in (3.5.3) for a suitable $\eta > 0$, so $\sum_{i=1}^{n} w_i(Y_i - \hat{\theta}_i) = 0$ and therefore $\underline{w}_k + \overline{w}_k = w_k$ when $Y_k \neq \hat{\theta}_k$.

- If (i) holds, then we can take $\theta = \hat{\theta} + \varepsilon\eta\mathbf{1}^{[1:k]}$ and $\theta = \hat{\theta} + \varepsilon\eta\mathbf{1}^{[k:n]}$ in (3.5.3) for some $\eta > 0$ and $\varepsilon \in \{-1, 1\}$, whence

$$-\varepsilon \sum_{i=k}^{n} w_i(Y_i - \hat{\theta}_i) = \varepsilon \sum_{i=1}^{k-1} w_i(Y_i - \hat{\theta}_i) \geq 0 \geq \varepsilon \sum_{i=1}^{k} w_i(Y_i - \hat{\theta}_i) = -\varepsilon \sum_{i=k+1}^{n} w_i(Y_i - \hat{\theta}_i). \tag{3.5.4}$$

  Thus, $\varepsilon w_k(\hat{\theta}_k - Y_k) \geq \varepsilon \sum_{i=1}^{k-1} w_i(Y_i - \hat{\theta}_i) \geq 0$, so $\underline{w}_k \in [0, w_k]$, and similarly $\overline{w}_k \in [0, w_k]$.

- Note that if $Y_k = \hat{\theta}_k$, then it follows from (3.5.4) that $\sum_{i=1}^{k-1} w_i(Y_i - \hat{\theta}_i) = 0 = \sum_{i=k+1}^{n} w_i(Y_i - \hat{\theta}_i)$.

- Under (ii), if $\theta = \hat{\theta} \pm \eta\mathbf{1}^{[1:k]} \in \Theta$ for some $\eta > 0$, then (3.5.3) implies that $\sum_{i=1}^{k} w_i(Y_i - \hat{\theta}_i) = 0 = \sum_{i=k+1}^{n} w_i(Y_i - \hat{\theta}_i)$, in which case $\overline{w}_k = 0$. The other case where $u = \mathbf{1}^{[k:n]}$ is similar.

(b) For each $k \in \{a,b\}$, either (i) or (ii) holds by hypothesis, so it follows from part (a) that $\underline{w}_k, \overline{w}_k \in [0,w_k]$ and $(\underline{w}_k + \overline{w}_k)(Y_k - \hat{\theta}_k) = w_k(Y_k - \hat{\theta}_k)$. Thus, defining $\tilde{w}^{1;a} := (w_1,\dots,w_{a-1},\underline{w}_a,0,\dots,0) \in \mathbb{R}^n$ and $\tilde{w}^{b;n} := (0,\dots,0,\overline{w}_b,w_{b+1},\dots,w_n) \in \mathbb{R}^n$, we have $\tilde{w}^{1;a},\tilde{w}^{a;b},\tilde{w}^{b;n} \in [0,\infty)^n$ and

$$w_i(Y_i - \hat{\theta}_i) = (\tilde{w}_i^{1;a} + \tilde{w}_i^{a;b} + \tilde{w}_i^{b;n})(Y_i - \hat{\theta}_i) \tag{3.5.5}$$

for $i \in [n]$. Moreover,

$$\sum_{i=1}^n \tilde{w}_i^{1;a}(Y_i - \hat{\theta}_i) = 0 = \sum_{i=1}^n \tilde{w}_i^{b;n}(Y_i - \hat{\theta}_i) \tag{3.5.6}$$

by the definitions of $\underline{w}_a, \overline{w}_b$ and the second bullet point above. Now for each $\theta \in \Theta \cup \{-\hat{\theta}\}$, we have $\hat{\theta} + \eta\theta^{(a:b)} \in \Theta$ for some $\eta > 0$ by assumption, so it follows from (3.5.3), (3.5.5) and (3.5.6) that

$$\begin{aligned} 0 \geq \sum_{i=1}^n w_i(Y_i - \hat{\theta}_i)\,\theta_i^{(a:b)} &= \sum_{i=1}^n \tilde{w}_i^{1;a}(Y_i - \hat{\theta}_i)\,\theta_a + \sum_{i=1}^n \tilde{w}_i^{a;b}(Y_i - \hat{\theta}_i)\,\theta_i + \sum_{i=1}^n \tilde{w}_i^{b;n}(Y_i - \hat{\theta}_i)\,\theta_b \\ &= \sum_{i=1}^n \tilde{w}_i^{a;b}(Y_i - \hat{\theta}_i)\,\theta_i \end{aligned}$$

for all $\theta \in \Theta \cup \{-\hat{\theta}\}$. In particular, this holds for $\theta = \pm\hat{\theta}$, so $\sum_{i=1}^n \tilde{w}_i^{a;b}(Y_i - \hat{\theta}_i)\,\hat{\theta}_i = 0$. We conclude that $\sum_{i=1}^n \tilde{w}_i^{a;b}(Y_i - \hat{\theta}_i)(\theta_i - \hat{\theta}_i) \leq 0$ for all $\theta \in \Theta$, and hence that $\hat{\theta} \in \operatorname{argmin}_{\theta \in \Theta} \|Y - \theta\|_{\tilde{w}^{a;b}}$ by (3.5.3), as required. □

For LSEs $\tilde{f}_n$ over classes $\tilde{\mathcal{F}}$ of shape-constrained functions on $[0,1]$, we will apply Lemma 3.5.1 to $\Theta \equiv \Theta(\tilde{\mathcal{F}}) := \bigl\{\bigl(f(x_1),\dots,f(x_n)\bigr) : 1 \leq i \leq n\bigr\}$ and $\hat{\theta} = \operatorname{argmin}_{\theta \in \Theta} \|Y - \theta\| = \bigl(\tilde{f}_n(x_1),\dots,\tilde{f}_n(x_n)\bigr)$, where $\|\cdot\|$ denotes the standard Euclidean norm on $\mathbb{R}^n$ corresponding to $w = \mathbf{1}$. The key observation is that the conditions in parts (a) and (b) of the lemma are satisfied when k (or a,b) is the index of a *jump* or *knot* of $\tilde{f}_n$. As mentioned previously, in our first setting of isotonic regression, Corollary 3.5.2 provides an alternative proof of a known result (e.g. Groeneboom and Jongbloed, 2014, Lemma 2.1); however, for the convex and S-shaped LSEs, treated in Corollary 3.5.3 and Proposition 3.5.4 respectively, the results are new to the best of our knowledge. Henceforth, for $f\colon [0,1] \to \mathbb{R}$ and a weight vector $w \equiv (w_1,\dots,w_n) \in [0,\infty)^n$, we write $S_n(f,w) := \sum_{i=1}^n w_i\bigl(Y_i - f(x_i)\bigr)^2$.

Corollary 3.5.2. *Let $\mathcal{F}^{\uparrow}$ denote the class of all non-decreasing functions $f\colon [0,1] \to \mathbb{R}$. Denote by $\bar{f}_n$ the (isotonic) LSE over $\mathcal{F}^{\uparrow}$ based on $\{(x_i,Y_i) : 1 \leq i \leq n\}$, which for definiteness is taken to be a left continuous, piecewise constant function with jumps only at the design points x_i. Let $1 \leq a \leq b \leq n$ be such that either $a = 1$ or $\bar{f}_n(x_{a-1}) < \bar{f}_n(x_a)$, and either $b = n$ or $\bar{f}_n(x_b) < \bar{f}_n(x_{b+1})$. Then $\bar{f}_n$ minimises $f \mapsto S_n(f,\mathbf{1}^{[a:b]}) = \sum_{i=a}^b \bigl(Y_i - f(x_i)\bigr)^2$ over $\mathcal{F}^{\uparrow}$, so that its restriction to $[x_a,x_b]$ coincides with the isotonic LSE based on $\{(x_i,Y_i) : a \leq i \leq b\}$.*

Proof. Here, $\Theta^{\uparrow} \equiv \Theta(\mathcal{F}^{\uparrow}) = \{\theta = (\theta_1,\dots,\theta_n) \in \mathbb{R}^n : \theta_1 \leq \cdots \leq \theta_n\}$ is the monotone cone, $w = \mathbf{1}$ is the weight vector and $\hat{\theta} = \operatorname{argmin}_{\theta \in \Theta^{\uparrow}} \|Y - \theta\| = \bigl(\bar{f}_n(x_1),\dots,\bar{f}_n(x_n)\bigr)$. Since $\hat{\theta} \pm \eta\mathbf{1}^{[a:n]} \in \Theta^{\uparrow}$ and $\hat{\theta} \pm \eta\mathbf{1}^{[1:b]} \in \Theta^{\uparrow}$ for all sufficiently small $\eta > 0$, condition (ii) of Lemma 3.5.1(a) holds for a,b. By Lemma 3.5.1(a), $\underline{w}_a = 0 = \overline{w}_b$, so $\tilde{w}^{a;b} = \mathbf{1}^{[a:b]}$. Since $\theta^{(a:b)} \in \Theta^{\uparrow}$ whenever $\theta \in \Theta$, we have $\hat{\theta} + \eta\theta^{(a:b)} \in \Theta^{\uparrow}$ for every $\eta > 0$, and moreover

$$\hat{\theta} + \eta(-\hat{\theta}^{(a:b)}) = \bigl(\hat{\theta}_1 - \eta\hat{\theta}_a,\dots,\hat{\theta}_{a-1} - \eta\hat{\theta}_a,(1-\eta)\hat{\theta}_a,\dots,(1-\eta)\hat{\theta}_b,\hat{\theta}_{b+1} - \eta\hat{\theta}_b,\dots,\hat{\theta}_n - \eta\hat{\theta}_b\bigr) \in \Theta^{\uparrow}$$

for every $\eta \in (0,1]$. We may therefore apply Lemma 3.5.1(b) to deduce the result. □

Corollary 3.5.3. *Let $\mathcal{C}$ denote the class of all convex functions $f\colon [0,1] \to \mathbb{R}$. Denote by $\breve{f}_n$ the (convex) LSE over $\mathcal{C}$ based on $\{(x_i,Y_i) : 1 \leq i \leq n\}$, which for definiteness is taken to an element of*

$\mathcal{G} \equiv \mathcal{G}[x_1, \dots, x_n]$. Let $1 \le a \le b \le n$ be such that for each $k \in \{a, b\}$, either $k \in \{1, n\}$ or x_k is a kink of $\breve{f}_n$. Let $\hat{\theta}_i := \breve{f}_n(x_i)$ for $i \in [n]$ and define $\tilde{w}^{a;b}$ in accordance with (3.5.1) and (3.5.2). Then $\breve{f}_n$ minimises $f \mapsto S_n(f, \tilde{w}^{a;b}) = \sum_{i=a}^{b} \tilde{w}_i^{a;b}\bigl(Y_i - f(x_i)\bigr)^2$ over $\mathcal{C}$.

Proof. Here, we take $\Theta \subseteq \mathbb{R}^n$ to be the closed, convex cone of convex sequences based on $x_1, \dots, x_n$, i.e.

$$\Theta(\mathcal{C}) = \left\{(\theta_1, \dots, \theta_n) \in \mathbb{R}^n : \frac{\theta_2 - \theta_1}{x_2 - x_1} \le \cdots \le \frac{\theta_n - \theta_{n-1}}{x_n - x_{n-1}}\right\}, \tag{3.5.7}$$

and $\hat{\theta} \equiv (\hat{\theta}_1, \dots, \hat{\theta}_n) = \mathrm{argmin}_{\theta \in \Theta} \|Y - \theta\|$. Observe that $\hat{\theta} + \eta\mathbf{1}^{[1:k]} \in \Theta$ and $\hat{\theta} + \eta\mathbf{1}^{[k:n]} \in \Theta$ for each $k \in \{a, b\}$ and sufficiently small $\eta > 0$, so condition (i) of Lemma 3.5.1(a) holds with $\varepsilon = 1$ for both a and b. Similar considerations to those in the proof of Corollary 3.5.2, but now with reference to the slopes $(\theta_i - \theta_{i-1})/(x_i - x_{i-1})$ for $i \in \{2, \dots, n\}$, reveal that $\hat{\theta} + \eta\theta^{(a:b)} \in \Theta$ for sufficiently small $\eta > 0$ and for every $\theta \in \Theta \cup \{-\hat{\theta}\}$. The result therefore follows again from Lemma 3.5.1(b). $\square$

When localising convex LSEs $\breve{f}_n$ to subintervals $[x_a, x_b]$ where a, b are kinks of $\breve{f}_n$, we usually require non-trivial boundary weights $\overline{w}_a, \underline{w}_b \in (0, 1)$, as defined in (3.5.1). We also mention that the conclusion of Corollary 3.5.3 remains valid if $\mathcal{C}$ is replaced throughout with $-\mathcal{C}$, the set of all concave functions $f \colon [0, 1] \to \mathbb{R}$. Indeed, this result for concave LSEs follows from essentially the same proof (taking $\varepsilon = -1$ instead in condition (i) of Lemma 3.5.1), or alternatively by a symmetry argument: if $\breve{f}_n$ is the LSE over $\mathcal{C}$ based on $\{(x_i, Y_i) : 1 \le i \le n\}$, then $-\breve{f}_n$ is the LSE over $-\mathcal{C}$ based on $\{(x_i, -Y_i) : 1 \le i \le n\}$.

The main result of this subsection of direct relevance for the rest of our work is Proposition 3.5.4 below, which reveals that the situation for localisation of S-shaped LSEs is more similar to that for convex LSEs than for isotonic LSEs, in that non-trivial boundary weights are generally required for localisation. Nevertheless, see also the examples following the proof for special cases where exact localisation holds. Recall the definition of $\mathcal{H}^m$ from Section 3.1.

Proposition 3.5.4. *For $m \in [0, 1]$, let $\hat{f}_n^m$ be the LSE over $\mathcal{H}^m$ based on $\{(x_i, Y_i) : i \in [n]\}$. For $j \in [n]$, let*

$$\underline{w}_j := \frac{\sum_{i=1}^{j-1}\bigl(Y_i - \hat{f}_n^m(x_i)\bigr)}{\hat{f}_n^m(x_j) - Y_j}\mathbb{1}_{\{\hat{f}_n^m(x_j) \ne Y_j\}} \quad \text{and} \quad \overline{w}_j := \frac{\sum_{i=j+1}^{n}\bigl(Y_i - \hat{f}_n^m(x_i)\bigr)}{\hat{f}_n^m(x_j) - Y_j}\mathbb{1}_{\{\hat{f}_n^m(x_j) \ne Y_j\}}, \tag{3.5.8}$$

similarly to (3.5.1). For $1 \le a \le b \le n$, define $\tilde{w}^{a;b} := (0, \dots, 0, \overline{w}_a, 1, \dots, 1, \underline{w}_b, 0, \dots, 0) \in \mathbb{R}^n$ similarly to (3.5.2), so that $\tilde{w}_i^{a;b} = 0$ for $1 \le i < a$ and $b < i \le n$ and $\tilde{w}_i^{a;b} = 1$ for $a < i < b$. If x_k, x_ℓ are knots of $\hat{f}_n^m$ with $x_{k+1} \le m \le x_{\ell-1}$, then $\tilde{w}^{1;k}, \tilde{w}^{k;\ell}, \tilde{w}^{\ell;n} \in [0, 1]^n$ and the following hold:

(a) $\hat{f}_n^m$ minimises $f \mapsto S_n(f, \tilde{w}^{1;k})$ over all $f \colon [0, 1] \to \mathbb{R}$ that are increasing and convex on $[x_1, x_k]$;

(b) $\hat{f}_n^m$ minimises $f \mapsto S_n(f, \tilde{w}^{\ell;n})$ over all $f \colon [0, 1] \to \mathbb{R}$ that are increasing and concave on $[x_\ell, x_n]$;

(c) $\hat{f}_n^m$ minimises $f \mapsto S_n(f, \tilde{w}^{k;\ell})$ over $\mathcal{H}^m$, and hence $S_n(\hat{f}_n^m, \tilde{w}^{k;\ell}) \le S_n(f, \tilde{w}^{k;\ell})$ for all $f \in \mathcal{F}^m$.

In addition, let x_K, x_L be the smallest and largest inflection points of $\hat{f}_n^m$ respectively.

(d) If $m \in (x_K, x_{K+1}]$, then $\underline{w}_K = 1$ and $\overline{w}_K = 0$. In this case, the increasing convex LSE $\hat{f}_{1,K}$ based on $\{(x_i, Y_i) : 1 \le i \le K\}$ agrees with $\hat{f}_n^m$ on $[x_1, x_K]$, and the increasing concave LSE $\hat{f}_{n,K+1}$ based on $\{(x_i, Y_i) : K+1 \le i \le n\}$ agrees with $\hat{f}_n^m$ on $[x_{K+1}, x_n]$.

(e) If $m \in [x_{L-1}, x_L)$, then $\underline{w}_L = 0$ and $\overline{w}_L = 1$. In this case, the increasing convex LSE $\hat{f}_{1,L-1}$ based on $\{(x_i, Y_i) : 1 \le i \le L-1\}$ agrees with $\hat{f}_n^m$ on $[x_1, x_{L-1}]$, and the increasing concave LSE $\hat{f}_{n,L}$ based on $\{(x_i, Y_i) : L \le i \le n\}$ agrees with $\hat{f}_n^m$ on $[x_L, x_n]$.

Proof. Here, $\Gamma^m := \Theta(\mathcal{F}^m) \subseteq \mathbb{R}^n$ is again a closed, convex cone, and $\hat{\theta} := \mathrm{argmin}_{\theta \in \Gamma^m} \|Y - \theta\| = \big(\hat{f}_n^m(x_1), \dots, \hat{f}_n^m(x_n)\big)$ corresponds to the weight vector $w = \mathbf{1}$. For k, ℓ as in (a, b, c), the facts $\tilde{w}^{1;k}, \tilde{w}^{k;\ell}, \tilde{w}^{\ell;n} \in [0,1]^n$ follow from Lemma 3.5.1(a), where it can be verified that condition (i) holds for k with $\varepsilon = 1$ and for ℓ with $\varepsilon = -1$. For (d, e), it can be seen that $\hat{\theta} \pm \eta \mathbf{1}^{[1:K]} \in \Gamma^m$ and $\hat{\theta} \pm \eta \mathbf{1}^{[L:n]} \in \Gamma^m$ for all sufficiently small $\eta > 0$, so condition (ii) in Lemma 3.5.1(a) holds and therefore $\underline{w}_K = 1$ and $\overline{w}_L = 1$. The remaining assertions in (a)–(e) then follow by checking the hypotheses of Lemma 3.5.1(b). □

Exact subinterval localisation: We now give some examples of situations where (d) and (e) hold, in which case the LSE $\hat{f}_n^m$ over $\mathcal{H}^m$ can be localised exactly to subintervals (without a non-trivial boundary adjustment) in the same way as for the isotonic LSE in Corollary 3.5.2. Let $s_n(j) := S_n(\hat{f}_n^{x_j})$ for each $j \in [n]$.

(i) If $K \in [n]$ is a *local* minimum of $j \mapsto s_n(j)$ satisfying $s_n(K-1) > s_n(K) = s_n(K+1)$, then (d) holds for $m = x_{K+1}$. Indeed, since $s_n(K-1) > s_n(K)$, we have $\hat{f}_n^{x_K} \notin \mathcal{H}^{x_{K-1}}$, so x_K must be the smallest inflection point of $\hat{f}_n^{x_K}$. Since $s_n(K) = s_n(K+1)$, it follows that $\hat{f}_n^{x_K} = \hat{f}_n^{x_{K+1}}$ minimises $f \mapsto S_n(f)$ over $\mathcal{H}^{x_K} \cup \mathcal{H}^{x_{K+1}}$, so the hypotheses of (d) are satisfied.

(ii) Similarly, if $L \in [n]$ is such that $s_n(L-1) = s_n(L) < s_n(L+1)$, then (e) holds for $m = x_{L-1}$.

(iii) If $\tilde{f}_n$ is an S-shaped LSE over $\mathcal{H} = \bigcup_{j=1}^n \mathcal{H}^{x_j}$ and x_K, x_L are its smallest and largest inflection points respectively, then when $m = x_{K+1}$, we have that (d) holds, and when $m = x_{L-1}$, we have that (e) holds. This yields the key Proposition 3.2.1 in Section 3.2.

3.5.2 A mixed primal-dual bases algorithm

In this subsection, we describe a mixed primal-dual bases algorithm the L^2-projection of a line segment onto the polyhedral convex cone of increasing convex sequences. This underpins our `SeqConReg` algorithm in Section 3.2. Our starting point is the following standard characterisation of projections onto general closed, convex cones (e.g. Groeneboom, 1996; Moreau, 1962, Corollary 2.1). Here and below, we write $\|\cdot\|$ and $\langle \cdot\,, \cdot \rangle$ for the standard Euclidean norm and inner product on $\mathbb{R}^n$ for some $n \in \mathbb{N}$.

Lemma 3.5.5. *Let $\Lambda \subseteq \mathbb{R}^n$ be a closed, convex cone. For each $y \in \mathbb{R}^n$, there exists a unique projection of y onto Λ, given by $\Pi_\Lambda(y) = \mathrm{argmin}_{u \in \Lambda} \|u - y\|$, and we have the following:*

(a) $\Pi_\Lambda(y)$ is the unique $\hat{y} \in \Lambda$ for which $\langle v, y - \hat{y} \rangle \le 0$ for all $v \in \Lambda$ and $\langle \hat{y}, y - \hat{y} \rangle = 0$.

(b) Suppose in addition that Λ is finitely generated, *i.e. that $\Lambda = \big\{\sum_{\ell=1}^r \lambda_\ell v^\ell : \lambda_1, \dots, \lambda_r \ge 0\big\}$ for some generators $v^1, \dots, v^r \in \Lambda$. Then $\hat{y} = \Pi_\Lambda(y)$ if and only if $\hat{y} = \sum_{\ell=1}^r \hat{\lambda}_\ell v^\ell$ for some $\hat{\lambda}_1, \dots, \hat{\lambda}_r \ge 0$, and $\langle v^\ell, y - \hat{y} \rangle \le 0$ for all ℓ, with $\langle v^\ell, y - \hat{y} \rangle = 0$ for any ℓ such that $\hat{\lambda}_\ell > 0$.*

In Lemma 3.5.5(b), the vector $(\hat{\lambda}_1, \dots, \hat{\lambda}_r)$ is the minimiser of a quadratic function $(\lambda_1, \dots, \lambda_r) \mapsto \|y - \sum_{\ell=1}^r \lambda_\ell v^\ell\|^2$ over the convex set $[0, \infty)^r$. When this constrained minimisation problem is written in Lagrangian form, the associated KKT optimality conditions (e.g. Rockafellar, 1997, Theorem 28.3) correspond precisely to the three conditions in (a) that uniquely define $\Pi_\Lambda(y)$, namely (i) $\hat{y} \in \Lambda$ (*primal feasibility*); (ii) $y - \hat{y} \in \{u \in \mathbb{R}^n : \langle u, v \rangle \le 0 \text{ for all } v \in \Lambda\}$, the *polar cone* of Λ (*dual feasibility*); and (iii) $\langle \hat{y}, y - \hat{y} \rangle = 0$ (*complementary slackness*).

Given $(x_1, Y_1), \dots, (x_n, Y_n) \in [0,1] \times \mathbb{R}$ with $x_1 < \cdots < x_n$, we now fix $j \in [n]$ and work with the cone Λ^j of increasing convex sequences based on $x_1, \dots, x_j$, as defined in (3.2.1). The projection of $(Y_1, \dots, Y_j)$ onto Λ^j is $\big(\hat{f}_{1,j}(x_1), \dots, \hat{f}_{1,j}(x_j)\big)$, where $\hat{f}_{1,j}$ is the increasing convex LSE based on $\{(x_i, Y_i) : i \in [j]\}$. The generators of Λ^j are $\pm u^0, u^1, \dots, u^{j-1} \in \mathbb{R}^j$, where $u^0 = \mathbf{1}$ and

$u_i^\ell = (x_i - x_\ell)^+$ for all $i \in [j]$ and $\ell \in [j-1]$. Since $u^0, u^1, \ldots, u^{j-1}$ are linearly independent, every $v \equiv (v_1, \ldots, v_j) \in \mathbb{R}^j$ can be represented uniquely in the form $v = \sum_{\ell=0}^{j-1} \lambda_\ell u^\ell$, where

$$\lambda_0 \equiv \lambda_0(v) = v_1; \quad \lambda_1 \equiv \lambda_1(v) = \frac{v_2 - v_1}{x_2 - x_1}; \quad \lambda_\ell \equiv \lambda_\ell(v) = \frac{v_{\ell+1} - v_\ell}{x_{\ell+1} - x_\ell} - \frac{v_\ell - v_{\ell-1}}{x_\ell - x_{\ell-1}}, \;\; 2 \leq \ell \leq j-1, \tag{3.5.9}$$

so that $v \in \Lambda^j$ if and only if $\lambda_\ell(v) \geq 0$ for all $\ell \in [j-1]$; this is the *primal feasibility* condition from Lemma 3.5.5. For each $v = \sum_{\ell=0}^{j-1} \lambda_\ell u^\ell \in \mathbb{R}^j$, the unique $g_v \in \mathcal{G}[x_1, \ldots, x_j]$ satisfying $v = \bigl(g_v(x_1), \ldots, g_v(x_j)\bigr)$ has a knot at x_ℓ if and only if $\lambda_\ell \neq 0$, so we refer to $A(v) := \{1 \leq \ell \leq j-1 : \lambda_\ell \neq 0\}$ as the set of *knots* of v (or 'active indices').

The following useful property of the projection map $\Pi_{\Lambda^j} : \mathbb{R}^j \to \Lambda^j$ can be derived easily from Lemma 3.5.5; see also Meyer and Woodroofe (2000, Proposition 1). A general version of this result for arbitrary closed, convex sets is stated as Lemma 3.6.1.

Lemma 3.5.6. *Let $A \subseteq [j-1]$ and $v', v'' \in \mathbb{R}^j$ be such that $A\bigl(\Pi_{\Lambda^j}(v)\bigr) = A$ for each $v \in \{v', v''\}$. Then for all $v \in [v', v''] := \{(1-t)v' + tv'' : t \in [0,1]\}$, we have $A\bigl(\Pi_{\Lambda^j}(v)\bigr) = A$ and, defining the linear subspace $\mathcal{L}_A := \operatorname{span}\{u^\ell : \ell \in A \cup \{0\}\} = \{v \in \mathbb{R}^j : A(v) \subseteq A\}$, we have $\Pi_{\Lambda^j}(v) = \Pi_{\mathcal{L}_A}(v)$.*

Remark 3.5.1. For $A \subseteq [j-1]$, the orthogonal projection onto the linear subspace $\mathcal{L}_A$ is represented by $P_A := U_A(U_A^\top U_A)^{-1} U_A^\top \in \mathbb{R}^{j \times j}$, where $U_A \in \mathbb{R}^{j \times (|A|+1)}$ is the matrix obtained by extracting the columns of $U := (u^0 \; u^1 \cdots u^{j-1}) \in \mathbb{R}^{j \times j}$ indexed by $A \cup \{0\}$. By taking $v' = v''$ in Lemma 3.5.6, we recover a version of Ghosal and Sen (2017, Proposition 2.1): suppose that we are given $v \in \mathbb{R}^j$ and have oracle knowledge of $A \equiv A\bigl(\Pi_{\Lambda^j}(v)\bigr)$, i.e. the locations of the knots of $\Pi_{\Lambda^j}(v)$. Then to compute $\Pi_{\Lambda^j}(v)$, we can note that $\Pi_{\Lambda^j}(v) = P_A v = \sum_{\ell=0}^{j-1} \hat{\lambda}_\ell u^\ell$, where $\hat{\lambda}_\ell \equiv \hat{\lambda}_\ell^A(v) := \lambda_\ell(P_A v)$ for $0 \leq \ell \leq j-1$, so that $\hat{\lambda}_\ell = 0$ for all $\ell \notin A$ and

$$\bigl(\hat{\lambda}_\ell : \ell \in A \cup \{0\}\bigr) = (U_A^\top U_A)^{-1} U_A^\top v = \underset{(\lambda_\ell \,:\, \ell \in A \cup \{0\})}{\operatorname{argmin}} \sum_{i=1}^n \Bigl(v_i - \lambda_0 - \sum_{\ell \in A} \lambda_\ell (x_i - x_\ell)^+\Bigr)^2 \tag{3.5.10}$$

solves an ordinary (*unconstrained*) least squares problem.

Observe now that if $v(0), v(1) \in \mathbb{R}^j$ are arbitrary and $v(t) := (1-t)v(0) + tv(1)$ for all $t \in (0,1)$, then $t \mapsto \Pi_{\Lambda^j}\bigl(v(t)\bigr)$ is a continuous, piecewise affine function from $[0,1]$ to Λ^j. Indeed, by Lemma 3.5.6 (and the continuity of projections onto closed, convex cones), there exist $0 = t_0' < t_1' < \cdots < t_{s+1}' = 1$ and distinct subsets $A_0', A_1', \ldots, A_s' \subseteq [j-1]$ such that for each $0 \leq r \leq s$, we have $\Pi_{\Lambda^j}\bigl(v(t)\bigr) = \Pi_{\mathcal{L}_{A_r'}}\bigl(v(t)\bigr) = P_{A_r'} v(t)$ for all $t \in [t_r', t_{r+1}']$.

Suppose that we are given $v(0), v(1) \in \mathbb{R}^j$ and the projection $\Pi_{\Lambda^j}\bigl(v(0)\bigr) \in \Lambda^j$, and now seek to compute $\Pi_{\Lambda^j}\bigl(v(1)\bigr)$. The reasoning in the previous paragraph suggests that we can proceed as in Algorithm 2.

Algorithm 2. Mixed primal-dual bases algorithm to compute projections onto the cone Λ^j.

(I) Starting at $t = t_0 := 0$, define $\hat{v}_0(t_0) := \Pi_{\Lambda^j}\bigl(v(0)\bigr)$ and let the initial active set be $A_0 := A\bigl(\hat{v}_0(t_0)\bigr)$, so that $\hat{v}_0(t_0) = \Pi_{\Lambda^j}\bigl(v(0)\bigr) = P_{A_0} v(0)$.

(II) For $r \in \mathbb{N}_0$, suppose inductively that at $t = t_r$, we are given that $\hat{v}_r(t_r) := \Pi_{\Lambda^j}\bigl(v(t_r)\bigr) = P_{A_r} v(t_r)$ for some $A_r \subseteq [j-1]$. Let $\hat{v}_r(t) := P_{A_r} v(t) = \hat{v}_r(t_r) - (t - t_r) P_{A_r} u$ for $t \in [t_r, 1]$, where $u := v(0) - v(1)$, and

$$t_{r+1} := \sup\bigl\{t \geq t_r : \lambda_\ell\bigl(\hat{v}_r(s)\bigr) \geq 0,\; \langle u^\ell, v(s) - \hat{v}_r(s) \rangle \leq 0 \text{ for all } s \in [t_r, t] \text{ and } \ell \in [j-1]\bigr\}. \tag{3.5.11}$$

By Lemma 3.5.5 and the fact that $\hat{v}_r(t_r) = \Pi_{\Lambda^j}\big(v(t_r)\big)$, the set on the right-hand side always contains t_r. In order to compute t_{r+1} explicitly, observe that for all $t \in [t_r, t_{r+1}]$, we have

(i) *Primal feasibility*: $\beta_\ell(t) := \lambda_\ell\big(\hat{v}_r(t)\big) = \lambda_\ell\big(\hat{v}_r(t_r) - (t-t_r)P_{A_r}u\big) = \beta_\ell(t_r) - (t - t_r)\,\lambda_\ell(P_{A_r}u) \geq 0$ for every $\ell \in [j-1]$, where equality holds if $\ell \in A_r^c$;

(ii) *Dual feasibility*: $\gamma_\ell(t) := \langle u^\ell, v(t) - \hat{v}_r(t)\rangle = \langle u^\ell, (I - P_{A_r})v(t)\rangle = \gamma_\ell(t_r) - (t - t_r)\,\hat{\zeta}_\ell^{A_r}(u) \leq 0$ for every $0 \leq \ell \leq j-1$, where equality holds if $\ell \in A_r \cup \{0\}$, and $\hat{\zeta}_\ell^{A_r}(u) := \langle u^\ell, (I - P_{A_r})u\rangle$.

In particular, $\beta_\ell(t), \gamma_\ell(t)$ depend linearly on $t \in [t_r, t_{r+1}]$, so

$$t_{r+1} = t_r + \min\left\{\frac{\beta_\ell(t_r)}{\hat{\lambda}_\ell^{A_r}(u)} : \ell \in [j-1],\, \hat{\lambda}_\ell^{A_r}(u) > 0\right\} \wedge \min\left\{\frac{\gamma_\ell(t_r)}{\hat{\zeta}_\ell^{A_r}(u)} : \ell \in A_r^c,\, \hat{\zeta}_\ell^{A_r}(u) < 0\right\} \tag{3.5.12}$$

since $\hat{\zeta}_\ell^{A_r}(u) = \langle (I - P_{A_r})u^\ell, u\rangle = 0$ for $\ell \in A_r \cup \{0\}$.

(iii) *Complementary slackness* is maintained throughout this step: $\langle \hat{v}_r(t), v(t) - \hat{v}_r(t)\rangle = \langle P_{A_r}v(t), (I - P_{A_r})v(t)\rangle = 0$, so $\Pi_{\Lambda^j}\big(v(t)\big) = \hat{v}_r(t) = P_{A_r}v(t)$ for all $t \in [t_r, t_{r+1}]$ by Lemma 3.5.5.

(III) If $t_{r+1} \geq 1$, then return $\hat{v}_r(1) = \hat{v}_r(t_r) - (1 - t_r)P_{A_r}u$ and terminate the algorithm. Otherwise, go to (IV), noting that when t approaches t_{r+1} from below, either

- A *primal variable* $\beta_\ell(t)$ with $\ell \in A_r$ is about to hit 0 and turn negative, or
- A *dual variable* $\gamma_\ell(t)$ with $\ell \in A_r^c$ is about to hit 0 and turn positive.

(IV) *Changing the 'active set'*: Define $A_r^- := \{\ell \in A_r : \beta_\ell(t_{r+1}) = 0\}$ and $A_r^+ := \{\ell \in A_r^c : \gamma_\ell(t_{r+1}) = 0\}$.

(a) If $|A_r^- \cup A_r^+| = 1$, then repeat (II) and (III) with $r+1$ in place of r and $A_{r+1} := (A_r \setminus A_r^-) \cup A_r^+$, observing that $\Pi_{\Lambda^j}\big(v(t_{r+1})\big) = P_{A_r}v(t_{r+1}) = P_{A_{r+1}}v(t_{r+1})$.

(b) If $|A_r^- \cup A_r^+| > 1$, i.e. there is a *degeneracy* at t_{r+1}, then choose $A^\pm \subseteq A_r^\pm$ and carry out (II) with $r+1$ in place of r and $A_{r+1} = (A_r \setminus A^-) \cup A^+$. In doing so, if (3.5.12) yields a strict increase in t, then let the algorithm continue from there and pass to (III). Otherwise, retry this for different pairs of subsets $A^\pm \subseteq A_r^\pm$ until we can move a strictly positive distance in the next iteration of (II).

When defining the primal variables $\beta_\ell(t)$ in (II), it is convenient here that every $v \in \Lambda^j$ has a unique primal representation, which in this case is given by (3.5.9). The same is true of any cone in $\mathbb{R}^j$ generated by $\pm\tilde{u}^0, \ldots, \pm\tilde{u}^{q-1}, \tilde{u}^q, \ldots, \tilde{u}^{j-1}$, for some linearly independent $\tilde{u}^0, \tilde{u}^1, \ldots, \tilde{u}^{j-1}$. Thus, Algorithm 2 is applicable to all such cones, provided that the 'active sets' are taken to be subsets of $\{q, q+1, \ldots, j-1\}$ (Fraser and Massam, 1989), so in particular, it can also be used to compute isotonic and convex LSEs (in a sequential manner, as described in Section 3.2). Indeed, the sequential application of this mixed primal-dual bases algorithm to the monotone cone $\Theta^\uparrow$ from the proof of Corollary 3.5.2 yields the widely-used, linear time 'pool adjacent violators' algorithm (PAVA) (Barlow et al., 1972). Moreover, with appropriate modifications, Algorithm 2 can be extended to general polyhedral cones (Meyer, 1999) and polyhedral convex sets.

Lemma 3.5.7. *Algorithm 2 always terminates after finitely many steps with the correct solution* $\Pi_{\Lambda^j}\bigl(v(1)\bigr)$.

This follows from (i)–(iii) in Stage (II) and the following two observations:

(iv) The algorithm does not get stuck at any of the thresholds t_r; i.e. when $t = t_r$ for some r, there is always a subsequent iteration of (II) that strictly increases t;

(v) At distinct thresholds t_r, the corresponding 'active sets' A_r are distinct subsets of $[j-1]$.

We will justify (iv) and (v) in Section 3.6.1, where we also exploit the specific structure of Λ^j to handle the degeneracies mentioned in Stage (IV)(b); see in particular modification (IV') and Proposition 3.6.2.

3.5.3 Proofs for Section 3.3

For $\theta \in \mathbb{R}^n$ and $J = \{a, a+1, \ldots, b\}$ with $1 \leq a \leq b \leq n$, we write $\theta_J := (\theta_i : i \in J)$ for the subvector indexed by J. We say that $u \equiv (u_a, u_{a+1}, \ldots, u_b)$ is a convex sequence (based on $x_a, x_{a+1}, \ldots, x_b$) if $u = \bigl(f(x_a), f(x_{a+1}), \ldots, f(x_b)\bigr)$ for some convex $f\colon [0,1] \to \mathbb{R}$, and define concave and affine sequences analogously. Denote by $K^J \equiv K^{a,b}$ the set of all convex sequences based on $x_a, \ldots, x_b$, which is a closed, convex cone; see (3.5.7). Recall from Section 3.5.1 the definitions of the monotone cone $\Theta^{\uparrow} = \{(\theta_1, \ldots, \theta_n) \in \mathbb{R}^n : \theta_1 \leq \cdots \leq \theta_n\}$ and the convex cone $\Gamma^m = \Theta(\mathcal{F}^m) = \bigl\{\bigl(f(x_1), \ldots, f(x_n)\bigr) : f \in \mathcal{F}^m\bigr\}$ for $m \in [0,1]$. Let $\Gamma := \Theta(\mathcal{F}) = \bigcup_{j=1}^n \Gamma^{x_j}$, so that if $\tilde{f}_n$ is an LSE over $\mathcal{F}$, then $\tilde{\theta}_n := \bigl(\tilde{f}_n(x_1), \ldots, \tilde{f}_n(x_n)\bigr) \in \operatorname{argmin}_{\theta \in \Gamma} \|Y - \theta\|$. Sometimes, we will write, e.g., $\Gamma \equiv \Gamma[\mathcal{D}]$ to emphasise the dependence on the set $\mathcal{D}$ of design points $x_1 < \cdots < x_n$. For a general closed, convex cone $\Lambda \subseteq \mathbb{R}^n$ and $\theta \in \mathbb{R}^n$, we write $T_\Lambda(\theta) := \{\lambda(v - \theta) : v \in \Lambda,\ \lambda \geq 0\}$ for the corresponding *tangent cone* at θ.

For fixed $n \in \mathbb{N}$, let $Y := (Y_1, \ldots, Y_n)$, $\theta_0 := \bigl(f_0(x_1), \ldots, f_0(x_n)\bigr)$ and $\xi := (\xi_1, \ldots, \xi_n)$, so that $Y = \theta_0 + \xi$ under the model (3.1.1).

Sharp oracle inequalities

Proof of Theorem 3.3.1. For a fixed $\theta \in \Gamma$, define $V(\theta) := \theta_n - \theta_1$, and for $r > 0$, let $\Gamma(\theta, r) \equiv \Gamma(\theta, r)[\mathcal{D}] := \{v \in \Gamma[\mathcal{D}] : \|v - \theta\| \leq r\}$. To prove (3.3.1), we claim that it suffices to find $r_*(\theta) > 0$ such that

$$\mathbb{E}\biggl(\sup_{v \in \Gamma(\theta, r_*(\theta))} |Z^\top (v - \theta)|\biggr) \leq \frac{r_*(\theta)^2}{2}, \tag{3.5.13}$$

where $Z \sim N_n(0, I_n)$. Indeed, by the sub-Gaussianity of the errors in Assumption 1, it then follows from Bellec (2018, Propositions 2.4, 6.3 and 6.4 and their proofs) that for every $t > 0$, we have

$$\|\tilde{\theta}_n - \theta_0\| \leq \|\theta - \theta_0\| + r_*(\theta) + \sqrt{8t}$$

with probability at least $1 - e^{-t}$.

First, we note that $\Gamma(\theta, r) \subseteq \Theta^{\uparrow}(\theta, r) := \{v \in \Theta^{\uparrow} : \|v - \theta\| \leq r\}$ for each $r > 0$ and deduce from the proof of Chatterjee (2014, Theorem 2.2) that if we set $r_{1,*}(\theta) := Cn^{1/6}\bigl(1 + V(\theta)\bigr)^{1/3}$ for a sufficiently large universal constant $C > 0$, then

$$\mathbb{E}\biggl(\sup_{v \in \Gamma(\theta, r_{1,*}(\theta))} |Z^\top (v - \theta)|\biggr) \leq \mathbb{E}\biggl(\sup_{v \in \Theta^{\uparrow}(\theta, r_{1,*}(\theta))} |Z^\top (v - \theta)|\biggr) \leq \frac{r_{1,*}(\theta)^2}{2};$$

see also (3.4) in Bellec (2018). Moreover, by taking $\tilde{C} \geq 1$ to be sufficiently large in Lemma 3.6.4, we see from (3.6.8) that (3.5.13) is satisfied if we take $r_*(\theta) = r_{2,*}(\theta) := C'(Rn)^{1/10}\bigl(1 + V(\theta)\bigr)^{1/5}$

for some suitably large universal constant $C' > 0$. The desired conclusion follows upon setting $r_*(\theta) := r_{1,*}(\theta) \wedge r_{2,*}(\theta)$. $\square$

As mentioned in Section 3.3, it is possible to modify the definition of R in Theorem 3.3.1 to yield further refinements for certain designs. In particular, for a set $\mathcal{D}$ of design points $x_1 < \cdots < x_n$, define $\tilde{R}(\mathcal{D}) := 1$ if $n = 1$, and otherwise inductively set

$$\tilde{R}(\mathcal{D}) := \frac{x_n - x_1}{\min_{2 \le i \le n}(x_i - x_{i-1})} \wedge \min_{\mathcal{D}_1, \ldots, \mathcal{D}_k} \left(\sum_{\ell=1}^{k} \tilde{R}(\mathcal{D}_\ell)^{1/5} \right)^5, \tag{3.5.14}$$

where the minimum is taken over all partitions of $\mathcal{D}$ into $k \ge 2$ non-empty sets $\mathcal{D}_1, \ldots, \mathcal{D}_k$. The proofs of Lemmas 3.6.5 and 3.6.6 reveal that we can replace R in Theorem 3.3.1 with $n^{-1}\tilde{R}(\{x_1, \ldots, x_n\})$, which, due to the minimum in the definition, is certainly no larger than R. This claim follows by partitioning the set $\mathcal{D}$ of design points, then finding, for each subset $\mathcal{D}_\ell$ in the partition, a good approximation to a given S-shaped function at the design points in $\mathcal{D}_\ell$, and finally constructing an overall approximation by linear interpolation. To see the advantages of this modified (albeit more complicated) definition of $\tilde{R}(\mathcal{D})$, consider first a perturbation of the equispaced design $x_i = i/n$ for $i \in [n]$, where we set $x_0 := (1-\delta)/n$ for some $\delta \in (0,1)$. Then our original quantity R is at least $1/(2\delta)$ when $n \ge 2$, whereas

$$\frac{1}{n+1}\tilde{R}(\{x_0, x_1, \ldots, x_n\}) \le \frac{1}{n+1}\bigl\{\tilde{R}(\{x_1, \ldots, x_n\})^{1/5} + \tilde{R}(\{x_0\})^{1/5}\bigr\}^5 \le \frac{1}{n+1}\bigl((n-1)^{1/5}+1\bigr)^5 \lesssim 1.$$

As another example, fix $k \in \mathbb{N}$, suppose for simplicity that n/k is an integer, and suppose further that

$$x_{\ell k + j} = \frac{(\ell + \delta_j)k}{n},$$

for $\ell = 0, 1, \ldots, (n/k) - 1$ and $j = 1, \ldots, k$, where $0 < \delta_1 < \cdots < \delta_k < 1/2$. Here, the design points can be partitioned into k groups, within each of which the points are equispaced, so

$$R \ge \frac{1}{2k \min_j(\delta_{j+1} - \delta_j)},$$

when $n \ge 2$, while

$$\frac{1}{n}\tilde{R}(\{x_1, \ldots, x_n\}) \le \frac{1}{n}\left(k \cdot \frac{n^{1/5}}{k^{1/5}}\right)^5 \wedge R = k^4 \wedge R.$$

Thus, in both examples, the modified definition may provide a significant improvement, in the first case when $\delta \ll 1$, and in the second, when $k^5 \ll 1/\min_j(\delta_{j+1} - \delta_j)$. This enables us to recover a rate of convergence of $n^{-2/5}$ in Theorem 3.3.1 in both cases, provided that k is treated as a constant in the second case. Overall, this new definition yields additional insight into the effect of the design on the rate of convergence, and provides reassurance about the robustness of the performance of the LSE $\hat{f}_n$ for much wider classes of designs.

Proof of Theorem 3.3.2. For a closed, convex cone $\Lambda \subseteq \mathbb{R}^n$, recall that the *statistical dimension* of Λ is defined as $\delta(\Lambda) := \mathbb{E}\bigl(\|\Pi_\Lambda(Z)\|^2\bigr)$, where $Z \sim N_n(0, I_n)$ and $\Pi_\Lambda \colon \mathbb{R}^n \to \Lambda$ denotes the projection map onto Λ (Amelunxen et al., 2014). Since Γ is the union of the closed, convex cones $\Gamma^{x_1}, \ldots, \Gamma^{x_n}$ and by Assumption 1, it follows from (2.7) and Propositions 6.1 and 6.4 of Bellec (2018) that for any $\theta \in \Gamma$ and $t > 0$, we have

$$\|\tilde{\theta}_n - \theta_0\| \le \|\theta - \theta_0\| + 2\left(\max_{1 \le j \le n} \delta^{1/2}\bigl(T_{\Gamma^{x_j}}(\theta)\bigr) + \sqrt{2(t + \log n)}\right) \tag{3.5.15}$$

with probability at least $1 - e^{-t}$. Denoting by k_θ the smallest $k \in \mathbb{N}$ for which $\theta \equiv (\theta_1, \ldots, \theta_n) \in \mathbb{R}^n$ is affine on k pieces, we claim that

$$\delta\big(T_{\Gamma^{x_j}}(\theta)\big) \le 8(k_\theta + 1)\log\biggl(\frac{en}{k_\theta + 1}\biggr)$$

for all $j \in [n]$ and $\theta \in \Gamma$. Indeed, for fixed $j \in [n]$ and $\theta \in \Gamma$, we write $k \equiv k_\theta$ and let $0 = j_0 \le j_1 < \cdots < j_{k'} = j < j_{k'+1} < \cdots < j_k < j_{k+1} = n$ be such that the subvector $\theta_{J_r} = (\theta_i : j_r + 1 \le i \le j_{r+1})$ indexed by $J_r := \{j_r + 1, j_r + 2, \ldots, j_{r+1}\}$ is an affine sequence for every $0 \le r \le k$. Then for any $v \in \Gamma^{x_j}$, note that $(v - \theta)_{J_r}$ is a convex sequence if $0 \le r \le k' - 1$ and a concave sequence if $k' \le r \le k$. Thus, $T_{\Gamma^{x_j}}(\theta) = \{\lambda(v - \theta) : v \in \Gamma^{x_j},\, \lambda \ge 0\} \subseteq \prod_{r=0}^{k'-1} K^{J_r} \times \prod_{r=k'}^{k} (-K^{J_r})$. Since $\delta(\pm K^{J_r}) \le 8\log(e|J_r|)$ for each $0 \le r \le k$ by Bellec (2018, Proposition 4.2), it follows from Amelunxen et al. (2014, Proposition 3.1(9, 10)) that

$$\delta\big(T_{\Gamma^{x_j}}(\theta)\big) \le \sum_{r=0}^{k'-1} \delta(K^{J_r}) + \sum_{r=k'}^{k} \delta(-K^{J_r}) \le \sum_{r=0}^{k} 8\log(e|J_r|) \le 8(k+1)\log\left(\frac{en}{k+1}\right), \tag{3.5.16}$$

as required, where the final inequality follows from Jensen's inequality and the fact that $\sum_{r=0}^{k} |J_r| = n$. Finally, if $f \in \mathcal{H}$ and $\theta = \big(f(x_1), \ldots, f(x_n)\big)$, then $\|f - f_0\|_n^2 = \|\theta - \theta_0\|^2/n$, so the sharp oracle inequality (3.3.3) is a direct consequence of (3.5.15) and (3.5.16). $\square$

Inflection point estimation

The proofs of some technical lemmas in this subsection are deferred to Section 3.6.2.

Proof of Theorem 3.3.3. For each $n \in \mathbb{N}$, let $\tilde{m}_- \equiv \tilde{m}_{n-}$ and $\tilde{m}_+ \equiv \tilde{m}_{n+}$ be the smallest and largest inflection points of $\tilde{f}_n$ respectively. Letting (C_n) be any deterministic positive sequence with $C_n \to \infty$, and defining the events $E_n^{\pm} := \big\{\pm(\tilde{m}_{\pm} - m_0) > C_n(n/\log n)^{-1/(2\alpha+1)}\big\}$, we aim to establish that $\mathbb{P}(E_n^{\pm}) \to 0$ as $n \to \infty$. We will consider only the events E_n^+; the arguments for E_n^- are analogous.

Our strategy is to show that there exist events (Ω_n) with $\mathbb{P}(\Omega_n^c) \to 0$ such that $\Delta_n := S_n(\tilde{f}_n) - S_n(\hat{f}_n^{m_0}) > 0$ on $E_n^+ \cap \Omega_n$ for all sufficiently large n. Since $\tilde{f}_n$ and $\hat{f}_n^{m_0}$ are LSEs over $\mathcal{F}$ and $\mathcal{H}^{m_0}$ respectively, we have $S_n(\tilde{f}_n) = \min_{f \in \mathcal{F}} S_n(f) \le S_n(\hat{f}_n^{m_0})$, so $E_n^+ \cap \Omega_n = \emptyset$ for all sufficiently large n, whence, by the reverse Fatou lemma, $\mathbb{P}(E_n^+) \le \mathbb{P}(E_n^+ \cap \Omega_n) + \mathbb{P}(\Omega_n^c) \to 0$, as desired.

Step 1 – subdividing $[0,1]$ and making 'boundary adjustments': For each n, we make the following definitions, suppressing the dependence on n to ease notation where appropriate. Writing $\hat{\tau}_- = x_\ell$ for the smallest inflection point of $\hat{f}_n^{m_0}$, we set $\hat{\tau}_L := \hat{\tau}_-$ if $\hat{\tau}_- < m_0$, and otherwise define $\hat{\tau}_L$ to be the largest knot of $\hat{f}_n^{m_0}$ in $[0, x_{\ell-1}]$. Also, let $\hat{\tau}_R$ be the smallest knot of $\hat{f}_n^{m_0}$ in $[\tilde{m}_+, 1]$. On the event E_n^+, we may decompose $[0,1]$ into the subintervals $\mathcal{I}_{-2} := [0, \hat{\tau}_L]$, $\mathcal{I}_{-1} := [\hat{\tau}_L, m_0)$, $\mathcal{I}_0 := [m_0, \tilde{m}_+]$, $\mathcal{I}_1 := (\tilde{m}_+, \hat{\tau}_R]$ and $\mathcal{I}_2 := [\hat{\tau}_R, 1]$. For $-2 \le A \le 2$, we associate $\mathcal{I}_A$ with a weight vector $w^A \in \mathbb{R}^n$ that is defined below in (3.5.17). Let $\hat{k}, \hat{\ell}$ be such that $\hat{\tau}_L = x_{\hat{\ell}}$ and $\hat{\tau}_R = x_{\hat{k}}$, and for $s \in \{\hat{k}, \hat{\ell}\}$, let

$$\underline{w}_s := \frac{\sum_{i=1}^{s-1}\big(Y_i - \hat{f}_n^{m_0}(x_i)\big)}{\hat{f}_n^{m_0}(x_s) - Y_s}\,\mathbb{1}_{\{\hat{f}_n^{m_0}(x_s) \ne Y_s\}} \quad \text{and} \quad \overline{w}_s := \frac{\sum_{i=s+1}^{n}\big(Y_i - \hat{f}_n^{m_0}(x_i)\big)}{\hat{f}_n^{m_0}(x_s) - Y_s}\,\mathbb{1}_{\{\hat{f}_n^{m_0}(x_s) \ne Y_s\}}$$

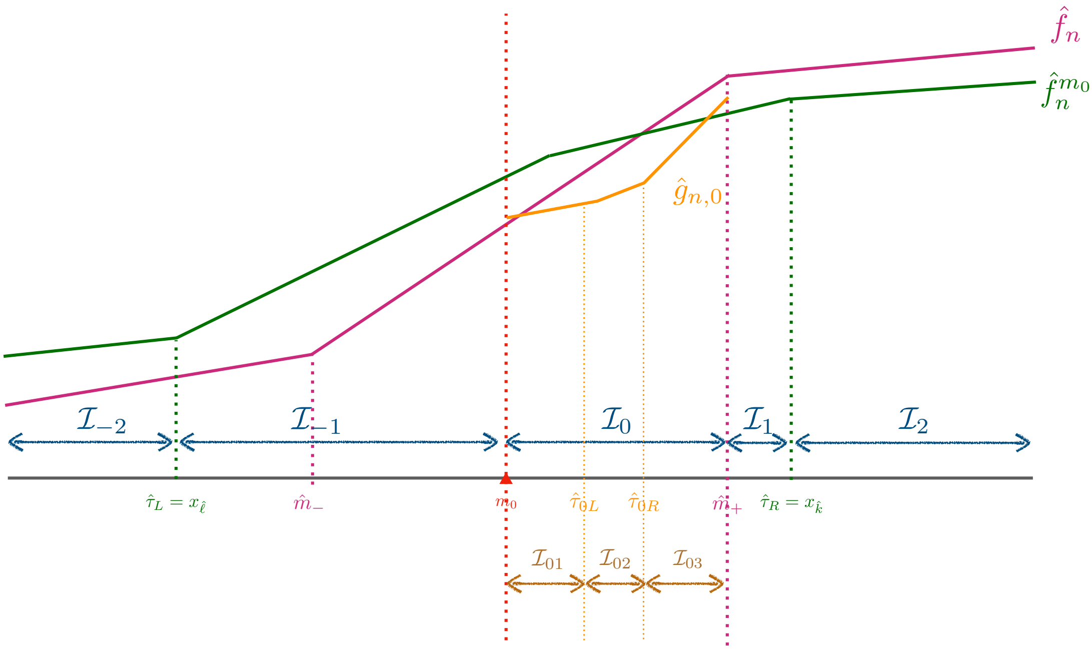

Figure 3.9: Illustration of the proof of Theorem 3.3.3.

as in (3.5.8), where $x_i \equiv x_{ni}$ and $Y_i \equiv Y_{ni}$ for all i. Then by Proposition 3.5.4, $\underline{w}_s, \overline{w}_s \in [0,1]$ and $\underline{w}_s + \overline{w}_s \leq 1$, with equality when $Y_s \neq \hat{f}_n^{m_0}(x_s)$. Now for $i \in [n]$ and $-2 \leq A \leq 2$, define

$$w_i^A := \begin{cases} 1 & \text{if } x_i \in \mathcal{I}_A \setminus \{\hat{k}, \hat{\ell}\} \\ 0 & \text{if } x_i \in \mathcal{I}_A^c \\ \underline{w}_i & \text{if either } A = -2 \text{ and } i = \hat{\ell}, \text{ or } A = 1 \text{ and } i = \hat{k} \\ \overline{w}_i & \text{if either } A = -1 \text{ and } i = \hat{\ell}, \text{ or } A = 2 \text{ and } i = \hat{k}. \end{cases} \tag{3.5.17}$$

Then $w^A \in [0,1]^n$ for all $-2 \leq A \leq 2$, and setting $S_n(f, w^A) := \sum_{i=1}^n w_i^A \bigl(Y_i - f(x_i)\bigr)^2$ for each $-2 \leq A \leq 2$ and $f\colon [0,1] \to \mathbb{R}$, we have

$$S_n(f) = \sum_{i=1}^n \bigl(Y_i - f(x_i)\bigr)^2 \geq \sum_{A=-2}^2 \sum_{i=1}^n w_i^A \bigl(Y_i - f(x_i)\bigr)^2 = \sum_{A=-2}^2 S_n(f, w^A),$$

with equality when $f = \hat{f}_n^{m_0}$. Thus, defining $\Delta_{n,A} := S_n(\tilde{f}_n, w^A) - S_n(\hat{f}_n^{m_0}, w^A)$ for $-2 \leq A \leq 2$, we see that $\Delta_n = S_n(\tilde{f}_n) - S_n(\hat{f}_n^{m_0}) \geq \sum_{A=-2}^2 \Delta_{n,A}$.

Since $\tilde{f}_n$ is increasing and convex on $\mathcal{I}_{-2}$ and increasing and concave on $\mathcal{I}_2$, it follows from Proposition 3.5.4 that $\Delta_{n,A} = S_n(\tilde{f}_n, w^A) - S_n(\hat{f}_n^{m_0}, w^A) \geq 0$ for each $A \in \{-2, 2\}$. Moreover, letting $w' := \sum_{A=-1}^1 w^A$, we have $\sum_{A=-1}^1 S_n(\hat{f}_n^{m_0}, w^A) = S_n(\hat{f}_n^{m_0}, w') \leq S_n(f_0, w') = \sum_{A=-1}^1 S_n(f_0, w^A)$ by Proposition 3.5.4(c) and the fact that $f_0 \in \mathcal{F}^{m_0}$. It is for these reasons that we made the 'boundary adjustments' at $\hat{k}$ and $\hat{\ell}$ in (3.5.17). We can now write

$$\Delta_n \geq \sum_{A=-2}^2 \Delta_{n,A} \geq \sum_{A=-1}^1 \Delta_{n,A} = \sum_{A=-1}^1 \bigl\{S_n(\tilde{f}_n, w^A) - S_n(\hat{f}_n^{m_0}, w^A)\bigr\} = \sum_{A=-1}^1 \tilde{\Delta}_{n,A}, \tag{3.5.18}$$

where

$$\tilde{\Delta}_{n,A} := S_n(\tilde{f}_n, w^A) - S_n(f_0, w^A) = \sum_{i : x_i \in \mathcal{I}_A} w_i^A \bigl\{\bigl(Y_i - \tilde{f}_n(x_i)\bigr)^2 - \xi_i^2\bigr\}$$

for $A \in \{-1, 0, 1\}$, and seek to bound each of these three terms from below.

Step 2 – bounding $\tilde{\Delta}_{n,0}$: On the event E_n^+, note that $\tilde{f}_n$ is convex on $\mathcal{I}_0 = [m_0, \tilde{m}_+]$ and f_0 is concave on $\mathcal{I}_0$. We will exploit this mismatch of shape constraints on $\mathcal{I}_0$ to obtain a suitable lower bound on $\tilde{\Delta}_{n,0}$. For each n, define $\hat{g}_{n,0} \colon \mathcal{I}_0 \to \mathbb{R}$ to be the convex LSE based on $\{(x_i, Y_i) : x_i \in \mathcal{I}_0\}$, which for definiteness is taken to be a continuous, piecewise linear function with knots in $\{x_1, \dots, x_n\} \cap \mathcal{I}_0$. Then $S_n(\tilde{f}_n, w^0) \geq S_n(\hat{g}_{n,0}, w^0)$ and

$$\tilde{\Delta}_{n,0} \geq S_n(\hat{g}_{n,0}, w^0) - S_n(f_0, w^0) = \sum_{i:x_i \in \mathcal{I}_0} \bigl\{\bigl(\xi_i + f_0(x_i) - \hat{g}_{n,0}(x_i)\bigr)^2 - \xi_i^2\bigr\} \tag{3.5.19}$$

in view of the definition of w^0 in (3.5.17). On E_n^+, let $\hat{\tau}_{0L}$ be the largest knot of $\hat{g}_{n,0}$ in $[m_0, (m_0 + \tilde{m}_+)/2]$, and on $(E_n^+)^c$, set $\hat{\tau}_{0L} = m_0$ for concreteness. Suppressing the dependence on n for convenience, we define $\mathcal{I}_{01} := (m_0, \hat{\tau}_{0L}]$, $\mathcal{I}_{02} := \bigl(\hat{\tau}_{0L}, (m_0 + \tilde{m}_+)/2\bigr)$ and $\mathcal{I}_{03} := \bigl[(m_0 + \tilde{m}_+)/2, \tilde{m}_+\bigr)$, and decompose the right-hand side of (3.5.19) as $\Lambda_{n1} + \Lambda_{n2} + \Lambda_{n3}$, where

$$\Lambda_{nj} := \sum_{i:x_i \in \mathcal{I}_{0j}} \bigl\{\bigl(\xi_i + f_0(x_i) - \hat{g}_{n,0}(x_i)\bigr)^2 - \xi_i^2\bigr\} \tag{3.5.20}$$

for $j \in \{1, 2, 3\}$. In the arguments below, a key ingredient is the following fact, whose proof (which we remind the reader is given in Section 3.6.2) makes use of Assumption 2.

Lemma 3.5.8. $\hat{\tau}_{0L} - m_0 = O_p\bigl((n/\log n)^{-1/(2\alpha+1)}\bigr)$.

Defining $t_n := \sqrt{C_n}\,(n/\log n)^{-1/(2\alpha+1)}$ and $u_n := 2^{-1}C_n(n/\log n)^{-1/(2\alpha+1)}$, we deduce that there are events (E_{n1}) with $\mathbb{P}(E_{n1}^c) \to 0$ such that $m_0 \leq \hat{\tau}_{0L} \leq m_0 + t_n$ and $(m_0 + \tilde{m}_+)/2 \geq m_0 + u_n$ on $E_n^+ \cap E_{n1}$, for each n.

Step 2a – bounding Λ_{n2}: For each n, note that by the definition of $\hat{\tau}_{0L}$, the function $\hat{g}_{n,0}$ is linear on $\mathcal{I}_{02} = \bigl(\hat{\tau}_{0L}, (m_0 + \tilde{m}_+)/2\bigr)$, whereas f_0 is concave on $\mathcal{I}_{02}$. In view of this and the fact that $\mathcal{I}_{02}$ length $(m_0 + \tilde{m}_+)/2 - \hat{\tau}_{0L} \geq u_n - t_n = u_n\bigl(1 + o(1)\bigr)$ on $E_n^+ \cap E_{n1}$, we would expect the approximation error $\sum_{i:x_i \in \mathcal{I}_{02}} \bigl(\hat{g}_{n,0}(x_i) - f_0(x_i)\bigr)^2$ to be 'large'; see Lemma 3.5.9 below. Together with the arguments in Steps 2b and 3, this will enable us to prove that the quantity Λ_{n2} is positive and dominates (in magnitude) all the other terms $\Lambda_{n1}, \Lambda_{n3}, \Delta_{n,\pm 1}$ in (3.5.18)–(3.5.20). This yields the eventual conclusion (3.5.35) that $\Delta_n > 0$ with high probability on E_n^+.

To handle the randomness of $\mathcal{I}_{02}$, let

$$\mathcal{T}_n := \bigl\{(a, b) : 1 \leq a \leq b \leq n,\, m_0 \leq x_a \leq m_0 + t_n,\, x_b \geq m_0 + u_n\bigr\},$$

and for $(a, b) \in \mathcal{T}_n$, define the vectors $\mathbf{1}^{a,b} := (1, 1, \dots, 1) \in \mathbb{R}^{b-a+1}$, $x^{a,b} := (x_a, x_{a+1}, \dots, x_b)$, $\xi^{a,b} := (\xi_a, \xi_{a+1}, \dots, \xi_b)$ and $\theta^{a,b} := \bigl(f_0(x_a), f_0(x_{a+1}), \dots, f_0(x_b)\bigr)$. Then on the event $E_n^+ \cap E_{n1}$, we have

$$\begin{aligned}
\Lambda_{n2} &\geq \inf_{c_0, c_1 \in \mathbb{R}} \sum_{i:x_i \in \mathcal{I}_{02}} \bigl\{\bigl(\xi_i + f_0(x_i) - c_0 - c_1 x_i\bigr)^2 - \xi_i^2\bigr\} \\
&\geq \inf_{(a,b) \in \mathcal{T}_n} \inf_{c_0, c_1 \in \mathbb{R}} \bigl\{\|\theta^{a,b} - c_0\mathbf{1}^{a,b} - c_1 x^{a,b}\|^2 - 2\,\bigl\langle \xi^{a,b}, c_0\mathbf{1}^{a,b} + c_1 x^{a,b} - \theta^{a,b}\bigr\rangle\bigr\}.
\end{aligned} \tag{3.5.21}$$

For $(a, b) \in \mathcal{T}_n$, denote by $\Pi_{a,b}\,\xi^{a,b} := \operatorname{argmin}_{v \in L^{a,b}} \|\xi^{a,b} - v\|$ the projection of $\xi^{a,b}$ onto the subspace $L^{a,b} := \operatorname{span}\{\theta^{a,b}, \mathbf{1}^{a,b}, x^{a,b}\}$, which has dimension $d \equiv d_{a,b} \leq 3$. Then

$$\sup_{c_0, c_1 \in \mathbb{R}} \frac{\bigl|\bigl\langle \xi^{a,b}, c_0\mathbf{1}^{a,b} + c_1 x^{a,b} - \theta^{a,b}\bigr\rangle\bigr|}{\|c_0\mathbf{1}^{a,b} + c_1 x^{a,b} - \theta^{a,b}\|} = \sup_{c_0, c_1 \in \mathbb{R}} \frac{\bigl|\bigl\langle \Pi_{a,b}\,\xi^{a,b}, c_0\mathbf{1}^{a,b} + c_1 x^{a,b} - \theta^{a,b}\bigr\rangle\bigr|}{\|c_0\mathbf{1}^{a,b} + c_1 x^{a,b} - \theta^{a,b}\|} \leq \|\Pi_{a,b}\,\xi^{a,b}\|. \tag{3.5.22}$$

Now let $\{v_1,\ldots,v_d\}$ be an orthonormal basis of $L^{a,b}$, so that $\|\Pi_{a,b}\,\xi^{a,b}\| = \bigl(\sum_{j=1}^d \langle \xi^{a,b}, v_j\rangle^2\bigr)^{1/2} \leq \sqrt{3}\max_{1\leq j\leq d}|\langle \xi^{a,b}, v_j\rangle|$. For each $j\in[d]$, we have $\mathbb{E}\bigl(e^{t\langle \xi^{a,b},v_j\rangle}\bigr) \leq e^{\|tv_j\|^2/2} = e^{t^2/2}$ for all $t\in\mathbb{R}$ by Assumption 2, so $\langle \xi^{a,b}, v_j\rangle$ is sub-Gaussian with parameter 1. Thus, for each $(a,b)\in\mathcal{T}_n$ and every $c>0$, we have

$$\mathbb{P}\left(\sup_{c_0,c_1\in\mathbb{R}} \frac{|\langle \xi^{a,b}, c_0\mathbf{1}^{a,b}+c_1x^{a,b}-\theta^{a,b}\rangle|}{\|c_0\mathbf{1}^{a,b}+c_1x^{a,b}-\theta^{a,b}\|} \geq \sqrt{6c\log n}\right) \leq \mathbb{P}\bigl(\|\Pi_{a,b}\,\xi^{a,b}\| \geq \sqrt{6c\log n}\bigr) \leq 6n^{-c}. \tag{3.5.23}$$

Since $|\mathcal{T}_n|<n^2$, we can take $c=3\ (>2)$ in (3.5.23) and apply a union bound to deduce from (3.5.21) that there are events (E_{n2}) with $\mathbb{P}(E_{n2}^c)\to 0$ such that

$$\Lambda_{n2} \geq \inf_{(a,b)\in\mathcal{T}_n}\ \inf_{c_0,c_1\in\mathbb{R}} \bigl\{\|\theta^{a,b}-c_0\mathbf{1}^{a,b}-c_1x^{a,b}\|^2 - 2\sqrt{18\log n}\,\|\theta^{a,b}-c_0\mathbf{1}^{a,b}-c_1x^{a,b}\|\bigr\} \tag{3.5.24}$$

on $E_n^+\cap E_{n1}\cap E_{n2}$, for each n. Note that the quadratic function $t\mapsto t^2-2t\sqrt{18\log n}$ attains its minimum at $t=\sqrt{18\log n}$ and is increasing on $[\sqrt{18\log n},\infty)$. In addition, using the local smoothness condition on f_0 in Assumption 2 and the fact that $x_b-x_a \geq u_n-t_n = 2^{-1}C_n(n/\log n)^{-1/(2\alpha+1)}\bigl(1+o(1)\bigr)$ for all $(a,b)\in\mathcal{T}_n$, we can show that there exists $\rho_\alpha>0$, depending only on α, such that the following holds:

Lemma 3.5.9. $\inf_{(a,b)\in\mathcal{T}_n}\inf_{c_0,c_1\in\mathbb{R}}\|\theta^{a,b}-c_0\mathbf{1}^{a,b}-c_1x^{a,b}\|^2 \geq \rho_\alpha B^2 n u_n^{2\alpha+1} \geq \rho_\alpha B^2(C_n/4)^{2\alpha+1}\log n$ *for all sufficiently large n.*

Since $C_n\to\infty$, this means that $\inf_{(a,b)\in\mathcal{T}_n}\inf_{c_0,c_1\in\mathbb{R}}\|\theta^{a,b}-c_0\mathbf{1}^{a,b}-c_1x^{a,b}\| \geq \sqrt{18\log n}$ for all sufficiently large n, so it follows from (3.5.24) that

$$\Lambda_{n2} \geq \rho_\alpha B^2\left(\frac{C_n}{4}\right)^{2\alpha+1}\log n - 2\sqrt{(18\log n)\,\rho_\alpha B^2\left(\frac{C_n}{4}\right)^{2\alpha+1}\log n} \geq \frac{\rho_\alpha B^2}{2}\left(\frac{C_n}{4}\right)^{2\alpha+1}\log n \tag{3.5.25}$$

on $E_n^+\cap E_{n1}\cap E_{n2}$, for all sufficiently large n.

Step 2b – bounding Λ_{n1} and Λ_{n3}: For each n, note that $\hat{g}_{n,0}-f_0$ is convex on $\mathcal{I}_{01} := (m_0,\hat{\tau}_{0L}]$ and $\mathcal{I}_{03} = \bigl[(m_0+\tilde{m}_+)/2, \tilde{m}_+\bigr)$. For $j=1,3$, writing $\tilde{g}_{nj}$ for the convex LSE based on $\{(x_i,\xi_i): x_i\in\mathcal{I}_{0j}\}$, we see from (3.5.20) that $\Lambda_{nj} \geq \sum_{i:x_i\in\mathcal{I}_{0j}}\bigl\{\bigl(\xi_i-\tilde{g}_{nj}(x_i)\bigr)^2-\xi_i^2\bigr\}$. To handle the randomness of $\mathcal{I}_{0j}$, let $\mathcal{T}_n' := \{(a,b): 1\leq a\leq b\leq n\}$ and for $(a,b)\in\mathcal{T}_n'$, denote by $\hat{\xi}^{a,b} := \operatorname{argmin}_{v\in K^{a,b}}\|\xi^{a,b}-v\|$ the projection of $\xi^{a,b} = (\xi_a,\xi_{a+1},\ldots,\xi_b)$ onto the closed, convex cone $K^{a,b}$ of convex sequences based on $x_a,\ldots,x_b$, as defined at the start of Section 3.5.3. Then $\|\xi^{a,b}\|^2 - \|\xi^{a,b}-\hat{\xi}^{a,b}\|^2 = \|\hat{\xi}^{a,b}\|^2$ by Lemma 3.5.5, and for every $c>0$, we have

$$\mathbb{P}\bigl\{\|\hat{\xi}^{a,b}\|^2 \geq 16\log\bigl(e(b-a+1)\bigr)+4c\log n\bigr\} \leq n^{-c}. \tag{3.5.26}$$

This can be seen by taking $\mu=u=0$ in Bellec (2018, Theorem 4.3), an oracle inequality for convex LSEs that holds under the sub-Gaussian condition on the errors in Assumption 2, in view of Bellec (2018, Remark 2.2, Proposition 6.2 and Proposition 6.4). Since $|\mathcal{T}_n'|<n^2$, we now take $c=3$ in (3.5.26) and apply a union bound to conclude that there are events (E_{n3}) with $\mathbb{P}(E_{n3}^c)\to 0$ such that

$$\begin{aligned}\Lambda_{nj} \geq \sum_{i:x_i\in\mathcal{I}_{0j}}\bigl\{\bigl(\xi_i-\tilde{g}_{nj}(x_i)\bigr)^2-\xi_i^2\bigr\} &\geq -\max_{(a,b)\in\mathcal{T}_n'}\bigl\{\|\xi^{a,b}-\hat{\xi}^{a,b}\|^2-\|\xi^{a,b}\|^2\bigr\}\\ &= -\max_{(a,b)\in\mathcal{T}_n'}\|\hat{\xi}^{a,b}\|^2 \geq -28\log(en)\end{aligned} \tag{3.5.27}$$

for $j = 1, 3$ on $E_n^+ \cap E_{n1} \cap E_{n3}$, for each n.

Step 3 – bounding $\tilde{\Delta}_{n,A}$ for $A \in \{-1, 1\}$: The techniques we apply here are broadly similar to those used in Step 2b, but the arguments are a little more involved. For each n, we now consider $\mathcal{I}_{-1} = [\hat{\tau}_L, m_0)$ and $\mathcal{I}_1 = (\tilde{m}_+, \hat{\tau}_R]$, where $\hat{\tau}_L = x_{\hat{\ell}}$ and $\hat{\tau}_R = x_{\hat{k}}$ are as given in Step 1. Let $\hat{\ell}_+, \hat{k}_- \in [n]$ be such that $x_{\hat{\ell}_+}$ is the smallest knot of $\hat{f}_n^{m_0}$ in $(\hat{\tau}_L, 1]$ and $x_{\hat{k}_-}$ is the largest knot of $\hat{f}_n^{m_0}$ in $[0, \hat{\tau}_R)$. Then $\{i : x_i \in \mathcal{I}_{-1}\} \subseteq \{\hat{\ell}, \hat{\ell}+1, \ldots, \hat{\ell}_+\}$ and $\{i : x_i \in \mathcal{I}_1\} \subseteq \{\hat{k}_-, \hat{k}_- + 1, \ldots, \hat{k}\}$ in all cases, in view of the definitions of $\hat{\tau}_L, \hat{\tau}_R$. Later on, we will apply Lemma 3.5.10 to $x_{\hat{\ell}}, x_{\hat{\ell}_+}$ and $x_{\hat{k}_-}, x_{\hat{k}}$, which are pairs of successive knots of $\hat{f}_n^{m_0}$.

Recalling from (3.5.18) that we defined $\tilde{\Delta}_{n,\pm 1}$ as weighted sums of squares, we start by bounding these from below by unweighted sums that do not feature the (random) 'boundary weights' $\underline{w}_{\hat{k}}, \overline{w}_{\hat{\ell}} \in [0,1]$ from (3.5.17). For $1 \le a \le b \le n$, let $K^{a,b}$ be as in Step 2b, so that $K^{a,b}$ and $-K^{a,b}$ are the cones of convex and concave sequences respectively based on $x_a, \ldots, x_b$, and let $\xi^{a,b} = (\xi_a, \xi_{a+1}, \ldots, \xi_b)$. Denote by $\check{\theta}^{a,b} := \mathrm{argmin}_{v \in K^{a,b}} \|Y^{a,b} - v\|$ and $\hat{\theta}^{a,b} := \mathrm{argmin}_{v \in -K^{a,b}} \|Y^{a,b} - v\|$ the projections of $Y^{a,b} := (Y_a, Y_{a+1}, \ldots, Y_b)$ onto $K^{a,b}$ and $-K^{a,b}$ respectively. Let $\hat{a} := \lfloor n\tilde{m}_+ \rfloor + 1$ and $\check{b} := \lceil nm_0 \rceil - 1$, so that $x_{\hat{a}-1} \le \tilde{m}_+ < x_{\hat{a}}$ and $x_{\check{b}} < m_0 \le x_{\check{b}+1}$, and define $\check{a}, \hat{b} \in [n]$ by

$$\check{a} := \begin{cases} \hat{\ell} & \text{if } \big(Y_{\hat{\ell}} - \tilde{f}_n(x_{\hat{\ell}})\big)^2 \le \xi_{\hat{\ell}}^2 \\ \hat{\ell}+1 & \text{otherwise} \end{cases} \quad \text{and} \quad \hat{b} := \begin{cases} \hat{k} & \text{if } \big(Y_{\hat{k}} - \tilde{f}_n(x_{\hat{k}})\big)^2 \le \xi_{\hat{k}}^2 \\ \hat{k}-1 & \text{otherwise.} \end{cases}$$

Then $[x_{\check{a}}, x_{\check{b}}] \subseteq \mathcal{I}_{-1}$ and $[x_{\hat{a}}, x_{\hat{b}}] \subseteq \mathcal{I}_1$, so $\hat{\ell} \le \check{a} \le \check{b} \le \hat{\ell}_+$ and $\hat{k}_- \le \hat{a} \le \hat{b} \le \hat{k}$. On the event E_n^+, the function $\tilde{f}_n$ is convex on $[x_{\check{a}}, x_{\check{b}}] \subseteq \mathcal{I}_{-1}$ and concave on $[x_{\hat{a}}, x_{\hat{b}}] \subseteq \mathcal{I}_1$, so it follows from the definitions above that

$$\tilde{\Delta}_{n,A} = \sum_{i : x_i \in \mathcal{I}_A} w_i^A \big\{\big(Y_i - \tilde{f}_n(x_i)\big)^2 - \xi_i^2\big\} \ge \begin{cases} \|Y^{\check{a},\check{b}} - \check{\theta}^{\check{a},\check{b}}\|^2 - \|\xi^{\check{a},\check{b}}\|^2 & \text{for } A = -1 \\ \|Y^{\hat{a},\hat{b}} - \hat{\theta}^{\hat{a},\hat{b}}\|^2 - \|\xi^{\hat{a},\hat{b}}\|^2 & \text{for } A = 1 \end{cases} \tag{3.5.28}$$

on E_n^+. Next, we develop these bounds further using some orthogonality properties and the oracle inequality stated as Bellec (2018, Theorem 4.3) once again, taking into account the randomness of $\check{a}, \check{b}, \hat{a}, \hat{b}$. For $1 \le a < b \le n$, let $\mathbf{1}^{a,b}, x^{a,b} \in \mathbb{R}^{b-a+1}$ and $\theta^{a,b} = \big(f_0(x_a), f_0(x_{a+1}) \ldots, f_0(x_b)\big)$ be as in Step 2a, and write $A^{a,b} := \mathrm{span}\{\mathbf{1}^{a,b}, x^{a,b}\}$ for the subspace of affine sequences of length $b - a + 1$ based on $x_a, x_{a+1}, \ldots, x_b$. Then $\bar{\theta}^{a,b} := \mathrm{argmin}_{v \in A^{a,b}} \|\theta^{a,b} - v\|$ satisfies $\langle \theta^{a,b} - \bar{\theta}^{a,b}, \theta^{a,b} - \theta \rangle = 0$ for all $\theta \in A^{a,b}$. Moreover, for all sufficiently small $\eta > 0$, we have $\check{\theta}^{a,b} \pm \eta(\check{\theta}^{a,b} - \bar{\theta}^{a,b}) \in K^{a,b}$ and $\hat{\theta}^{a,b} \pm \eta(\hat{\theta}^{a,b} - \bar{\theta}^{a,b}) \in -K^{a,b}$, so it follows from (3.5.3) or Lemma 3.6.1(a) that $\langle Y^{a,b} - \check{\theta}^{a,b}, \bar{\theta}^{a,b} - \check{\theta}^{a,b} \rangle = 0$ and $\langle Y^{a,b} - \hat{\theta}^{a,b}, \bar{\theta}^{a,b} - \hat{\theta}^{a,b} \rangle = 0$. Therefore, writing $Y^{a,b} = \theta^{a,b} + \xi^{a,b}$, we deduce that

$$\begin{aligned} \|Y^{a,b} - \check{\theta}^{a,b}\|^2 - \|\xi^{a,b}\|^2 &= \|Y^{a,b} - \bar{\theta}^{a,b}\|^2 - \|\check{\theta}^{a,b} - \bar{\theta}^{a,b}\|^2 - \|\xi^{a,b}\|^2 \\ &= \|\xi^{a,b} + (\theta^{a,b} - \bar{\theta}^{a,b})\|^2 - \|\xi^{a,b}\|^2 - \|\check{\theta}^{a,b} - \bar{\theta}^{a,b}\|^2 \\ &= 2\,\langle \xi^{a,b}, \theta^{a,b} - \bar{\theta}^{a,b} \rangle - \|\check{\theta}^{a,b} - \bar{\theta}^{a,b}\|^2 + \|\theta^{a,b} - \bar{\theta}^{a,b}\|^2 \\ &\ge 2\,\langle \xi^{a,b}, \theta^{a,b} - \bar{\theta}^{a,b} \rangle - 2\,\|\check{\theta}^{a,b} - \theta^{a,b}\|^2 - \|\theta^{a,b} - \bar{\theta}^{a,b}\|^2, \end{aligned} \tag{3.5.29}$$

where the final inequality follows since $\|z + z'\|^2 \le 2(\|z\|^2 + \|z'\|^2)$ for $z, z' \in \mathbb{R}^{b-a+1}$. Similarly,

$$\|Y^{a,b} - \hat{\theta}^{a,b}\|^2 - \|\xi^{a,b}\|^2 \ge 2\,\langle \xi^{a,b}, \theta^{a,b} - \bar{\theta}^{a,b} \rangle - 2\,\|\hat{\theta}^{a,b} - \theta^{a,b}\|^2 - \|\theta^{a,b} - \bar{\theta}^{a,b}\|^2,$$

and we now address each of the three terms on the right-hand side in turn. Firstly, letting $v^{a,b} := (\theta^{a,b} - \bar{\theta}^{a,b}) / \|\theta^{a,b} - \bar{\theta}^{a,b}\|$, we have $\|v^{a,b}\| = 1$, so $\langle \xi^{a,b}, v^{a,b} \rangle$ is sub-Gaussian with parameter

1. Therefore, for any a, b with $1 \leq a \leq b \leq n$ and for every $c > 0$, we have

$$\mathbb{P}\bigl(|\langle \xi^{a,b}, \theta^{a,b} - \bar{\theta}^{a,b}\rangle| \geq \sqrt{2c\log n}\,\|\theta^{a,b} - \bar{\theta}^{a,b}\|\bigr) \leq 2n^{-c}. \tag{3.5.30}$$

Secondly, by taking $\mu = \theta^{a,b}$ and $u = \bar{\theta}^{a,b} \in A^{a,b}$ in Bellec (2018, Theorem 4.3) and applying this result to the closed, convex cones $\pm K^{a,b}$, we find that

$$\mathbb{P}\bigl\{\|\check{\theta}^{a,b} - \theta^{a,b}\|^2 \vee \|\hat{\theta}^{a,b} - \theta^{a,b}\|^2 \geq \|\theta^{a,b} - \bar{\theta}^{a,b}\|^2 + 16\log\bigl(e(b-a+1)\bigr) + 4c\log n\bigr\} \leq 2n^{-c} \tag{3.5.31}$$

for any a, b with $1 \leq a \leq b \leq n$ and for every $c > 0$. Finally, we can establish the following for each n (without using the local smoothness condition on f_0 in Assumption 2):

Lemma 3.5.10. *For $1 \leq a \leq b \leq n$, define $\check{\theta}^{a,b} := \bigl(\hat{f}_n^{m_0}(x_a), \hat{f}_n^{m_0}(x_{a+1}), \ldots, \hat{f}_n^{m_0}(x_b)\bigr)$, and as in Step 2a, let $\Pi_{a,b}\,\xi^{a,b} := \operatorname{argmin}_{v \in L^{a,b}} \|\xi^{a,b} - v\|$ be the projection of $\xi^{a,b}$ onto the subspace $L^{a,b} = \operatorname{span}\{\theta^{a,b}, \mathbf{1}^{a,b}, x^{a,b}\}$. If $x_{\tilde{k}} < x_{\tilde{k}'}$ are successive knots of $\hat{f}_n^{m_0}$, then*

$$\|\theta^{\tilde{k},\tilde{k}'} - \check{\theta}^{\tilde{k},\tilde{k}'}\| \leq \max_{1\leq a\leq b\leq n} \|\Pi_{a,b}\,\xi^{a,b}\| + 2\max_{1\leq i\leq n}|\xi_i| + 2\max_{1\leq i\leq n}|(\hat{f}_n^{m_0} - f_0)(x_i)| =: \Xi.$$

At the start of Step 3, $x_{\hat{\ell}}, x_{\hat{\ell}_+}$ and $x_{\hat{k}_-}, x_{\hat{k}}$ were defined to be pairs of successive knots of $\hat{f}_n^{m_0}$. Therefore, since $\hat{\ell} \leq \check{a} \leq \check{b} \leq \hat{\ell}_+$ and $\bigl(\check{\theta}_i^{\hat{\ell},\hat{\ell}_+}(x_{\check{a}}), \ldots, \check{\theta}_i^{\hat{\ell},\hat{\ell}_+}(x_{\check{b}})\bigr) \in A_{\check{a},\check{b}}$, it follows that

$$\|\theta^{\check{a},\check{b}} - \bar{\theta}^{\check{a},\check{b}}\|^2 = \min_{\theta \in A_{\check{a},\check{b}}} \|\theta^{\check{a},\check{b}} - \theta\|^2 \leq \sum_{i=\check{a}}^{\check{b}} \bigl(\theta_i^{\hat{\ell},\hat{\ell}_+} - \check{\theta}_i^{\hat{\ell},\hat{\ell}_+}\bigr)^2 \leq \|\theta^{\hat{\ell},\hat{\ell}_+} - \check{\theta}^{\hat{\ell},\hat{\ell}_+}\|^2 \leq \Xi^2.$$

Similarly, $\|\theta^{\hat{a},\hat{b}} - \bar{\theta}^{\hat{a},\hat{b}}\| \leq \|\theta^{\hat{k}_-,\hat{k}} - \check{\theta}^{\hat{k}_-,\hat{k}}\| \leq \Xi$. Now recall the tail bound (3.5.23) for $\|\Pi_{a,b}\,\xi^{a,b}\|$, which applies to all $1 \leq a \leq b \leq n$, and our Assumption 2 that $\xi_1, \ldots, \xi_n$ are sub-Gaussian random variables with parameter 1. Applying a union bound, we see that

$$\begin{aligned}\mathbb{P}\Bigl(&\max_{1\leq a\leq b\leq n}\|\Pi_{a,b}\,\xi^{a,b}\| + 2\max_{1\leq i\leq n}|\xi_i| \geq 6\sqrt{c\log n}\Bigr)\\ &\leq \mathbb{P}\Bigl(\max_{1\leq a\leq b\leq n}\|\Pi_{a,b}\,\xi^{a,b}\| \geq \sqrt{6c\log n}\Bigr) + \mathbb{P}\Bigl(\max_{1\leq i\leq n}|\xi_i| \geq \sqrt{2c\log n}\Bigr) \leq 6n^{2-c} + 2n^{1-c}\end{aligned}$$

for every $c > 0$. Since $\max_{x\in[0,1]}|(\hat{f}_n^{m_0} - f_0)(x)| = o_p(1)$ by Proposition 3.1.2(c), it follows from Lemma 3.5.10 that

$$\mathbb{P}\bigl(\|\theta^{\check{a},\check{b}} - \bar{\theta}^{\check{a},\check{b}}\| \vee \|\theta^{\hat{a},\hat{b}} - \bar{\theta}^{\hat{a},\hat{b}}\| \geq 6\sqrt{c\log n} + \eta\bigr) \leq \mathbb{P}\bigl(\Xi \geq 6\sqrt{c\log n} + \eta\bigr) \to 0 \tag{3.5.32}$$

as $n \to \infty$, for any $c > 2$ and $\eta > 0$. We now combine (3.5.32) with (3.5.30) and (3.5.31), where we take $c = 3$ (> 2) and apply a union bound to handle all pairs (a, b) with $1 \leq a \leq b \leq n$. Together with (3.5.28) and (3.5.29), these imply that there exist a universal constant $\rho' > 0$ and events (E_{n4}) with $\mathbb{P}(E_{n4}^c) \to 0$ such that

$$\begin{aligned}\tilde{\Delta}_{n,-1} \geq \|Y^{\check{a},\check{b}} - \check{\theta}^{\check{a},\check{b}}\|^2 - \|\xi^{\check{a},\check{b}}\|^2 &\geq 2\,\langle \xi^{\check{a},\check{b}}, \theta^{\check{a},\check{b}} - \bar{\theta}^{\check{a},\check{b}}\rangle - 2\,\|\check{\theta}^{\check{a},\check{b}} - \theta^{\check{a},\check{b}}\|^2 - \|\theta^{\check{a},\check{b}} - \bar{\theta}^{\check{a},\check{b}}\|^2\\ &\geq -2\sqrt{2\log n}\,\|\theta^{\check{a},\check{b}} - \bar{\theta}^{\check{a},\check{b}}\| - 56\log(en) - 3\,\|\theta^{\check{a},\check{b}} - \bar{\theta}^{\check{a},\check{b}}\|^2\\ &\geq -\rho'\log(en)\end{aligned} \tag{3.5.33}$$

and

$$
\begin{aligned}
\tilde{\Delta}_{n,1} \geq \|Y^{\hat{a},\hat{b}} - \hat{\theta}^{\hat{a},\hat{b}}\|^2 - \|\xi^{\hat{a},\hat{b}}\|^2 &\geq 2\,\langle \xi^{\hat{a},\hat{b}}, \theta^{\hat{a},\hat{b}} - \bar{\theta}^{\hat{a},\hat{b}}\rangle - 2\,\|\hat{\theta}^{\hat{a},\hat{b}} - \theta^{\hat{a},\hat{b}}\|^2 - \|\theta^{\hat{a},\hat{b}} - \bar{\theta}^{\hat{a},\hat{b}}\|^2 \\
&\geq -2\sqrt{2\log n}\,\|\theta^{\hat{a},\hat{b}} - \bar{\theta}^{\hat{a},\hat{b}}\| - 56\log(en) - 3\,\|\theta^{\hat{a},\hat{b}} - \bar{\theta}^{\hat{a},\hat{b}}\|^2 \\
&\geq -\rho'\log(en) \qquad (3.5.34)
\end{aligned}
$$

on $E_n^+ \cap E_{n1} \cap E_{n4}$, for each n.

Having carried out Steps 1–3 above, we finally define the events $\Omega_n := \bigcap_{j=1}^4 E_{nj}$ for $n \in \mathbb{N}$, which satisfy $\mathbb{P}(\Omega_n^c) \to 0$. We conclude from (3.5.18), (3.5.25), (3.5.27), (3.5.33) and (3.5.34) that

$$
\begin{aligned}
\Delta_n = S_n(\tilde{f}_n) - S_n(\hat{f}_n^{m_0}) &\geq \sum_{A=-1}^{1} \tilde{\Delta}_{n,A} = \Lambda_{n2} + \Lambda_{n1} + \Lambda_{n3} + \tilde{\Delta}_{n,-1} + \tilde{\Delta}_{n,1} \qquad (3.5.35) \\
&\geq 2^{-1}\rho_\alpha B^2\,(C_n/4)^{2\alpha+1}\log n - 2\,(28\log n) - 2\rho'\log(en) > 0
\end{aligned}
$$

on $E_n^+ \cap \Omega_n$, for all sufficiently large n. As mentioned at the start of the proof, this means that $\mathbb{P}(E_n^+) \leq \mathbb{P}(E_n^+ \cap \Omega_n) + \mathbb{P}(\Omega_n^c) \to 0$, as desired. □

Proof of Proposition 3.3.4. Fix $\tau \in (0,1)$. First, we consider the case where $f_0 \in \mathcal{F}^{m_0}$ satisfies Assumption 2 for some $\alpha > 1$. By suitably perturbing f_0, we construct for each (sufficiently large) n a function $f_{\delta_n} \in \mathcal{F}(f_0, \tau/\sqrt{n})$ that has a unique inflection point at distance of order $\delta_n \asymp (\tau^2/n)^{1/(2\alpha+1)}$ from m_0. The local asymptotic minimax lower bound (3.3.6) is then obtained by applying (the proof of) Le Cam's two-point lemma to $\{f_0, f_{\delta_n}\}$. We will write $d_{\mathrm{TV}}(P,Q)$ for the total variation distance between probability measures P, Q.

To this end, for each $\delta \in (0, 1-m_0)$, let $u(m_0+\delta)$ be a subgradient of the concave function $f_0|_{[m_0,1]}$ at $m_0+\delta$, so that $u(m_0+\delta) < f_0'(m_0)$ and

$$
f_0(x) \leq f_0(m_0+\delta) + u(m_0+\delta)(x - m_0 - \delta) =: f_{1,\delta}(x) \quad \text{for all } x \in [m_0, 1].
$$

Define

$$
f_{2,\delta}(x) := f_0(m_0) + f_0'(m_0)(x-m_0) + \delta(x-m_0)^\alpha \quad \text{for } x \in [m_0,1],
$$

so that $f_{2,\delta}$ is strictly convex on $[m_0,1]$ (thanks to the inclusion of the final term $\delta(x-m_0)^\alpha$) and $f_{2,\delta}(x) > f_0(m_0) + f_0'(m_0)(x-m_0) \geq f_0(x)$ for all $x \in (m_0,1]$. Note in particular that $f_{1,\delta}(m_0) > f_0(m_0) = f_{2,\delta}(m_0)$ and $f_{1,\delta}(m_0+\delta) = f_0(m_0+\delta) < f_{2,\delta}(m_0+\delta)$. Consequently, defining $f_\delta \colon [0,1] \to \mathbb{R}$ by

$$
f_\delta(x) := \begin{cases} f_0(x) & x \in [0,m_0] \cup [m_0+\delta, 1] \\ f_{1,\delta}(x) \wedge f_{2,\delta}(x) & x \in (m_0, m_0+\delta), \end{cases} \qquad (3.5.36)
$$

we deduce that there exists a unique $c_\delta \in (0,1)$ such that $f_\delta = f_{2,\delta}$ on $[m_0, m_0+\delta c_\delta]$ and $f_\delta = f_{1,\delta}$ on $[m_0+\delta c_\delta, m_0+\delta]$. Moreover, since $f_{2,\delta}$ is strictly convex and $f_{1,\delta}(m_0+\delta c_\delta) > f_0'(m_0) > u(m_0+\delta) = f_{2,\delta}(m_0+\delta c_\delta)$, it follows that f_δ lies in $\mathcal{F}$ and has a unique inflection point at $m_\delta := m_0 + \delta c_\delta$.

Now for any sequence (δ_n) with $\delta_n \to 0$ and $n\delta_n \to \infty$, it follows from Assumption 2 and some elementary analytic arguments that the following holds as $n \to \infty$; see Section 3.6.2.

Lemma 3.5.11. *For $\alpha > 1$, we have $\|f_{\delta_n} - f_0\|_n^2 = \big(1+o(1)\big)\int_0^1 (f_{\delta_n} - f_0)^2 = \big(1+o(1)\big)C_\alpha B^2 \delta_n^{2\alpha+1}$ and $c_{\delta_n} = \big(1+o(1)\big)(1-\alpha^{-1})$ as $n \to \infty$, where $C_\alpha := \int_0^1 \big\{t^\alpha - \big(1-(1-t)\alpha\big)^+\big\}^2\,dt > 0$.*

Thus, setting $\delta_n := \big(1+o(1)\big)(2C_\alpha B^2 n\tau^{-2})^{-1/(2\alpha+1)}$, we deduce that $f_{\delta_n} \in \mathcal{F}(f_0, \tau/\sqrt{n})$ for all sufficiently large n. For all such n, write $P_{0,n}^Y, P_{1,n}^Y$ for the distributions of $(Y_{n1}, \ldots, Y_{nn})$ under the data generating mechanisms $Y_{ni} = f_0(x_{ni}) + \xi_{ni}$ and $Y_{ni} = f_{\delta_n}(x_{ni}) + \xi_{ni}$ respectively. Since

$\xi_{n1},\ldots,\xi_{nn} \overset{\text{iid}}{\sim} N(0,1)$ by assumption, we have by Pinsker's inequality that $d_{\mathrm{TV}}^2(P_{0,n}^Y, P_{1,n}^Y) \leq \mathrm{KL}(P_{0,n}^Y, P_{1,n}^Y)/2 = n\|f_{\delta_n} - f_0\|_n^2/2$, so for all sufficiently large n, the minimax risk can be bounded from below using Le Cam's two point lemma:

$$\begin{aligned}\inf_{\check{m}_n} \sup_{f\in\mathcal{F}(f_0,\tau/\sqrt{n})} \mathbb{E}_f\bigl(d(\check{m}_n, \mathcal{I}_f)\bigr) &\geq \frac{1}{2}\inf_{\check{m}_n}\{\mathbb{E}_{f_0}(|\check{m}_n - m_0|) + \mathbb{E}_{f_{\delta_n}}(|\check{m}_n - m_{\delta_n}|)\}\\ &\geq \frac{|m_{\delta_n} - m_0|}{2}\bigl(1 - d_{\mathrm{TV}}(P_{0,n}^Y, P_{1,n}^Y)\bigr)\\ &\geq \bigl(1 + o(1)\bigr)\,\frac{\alpha-1}{2\alpha}\biggl(\frac{2C_\alpha B^2 n}{\tau^2}\biggr)^{-1/(2\alpha+1)}\biggl(1 - \frac{\tau}{2^{1/2}}\biggr).\end{aligned}$$

This yields (3.3.6), as desired.

In the case $\alpha \in (0,1)$, we instead define $f_\delta\colon [0,1] \to \mathbb{R}$ for $\delta \in (0, 1-m_0)$ by

$$f_\delta(x) = \begin{cases} f_0(x) \wedge \bigl\{f_0(m_0) + (1-\delta)\frac{f_0(m_0+\delta) - f_0(m_0)}{\delta}(x - m_0)\bigr\} & \text{for } x \in [0, m_0]\\ f_0(m_0) + \bigl(f_0(m_0+\delta) - f_0(m_0)\bigr)\bigl\{(1-\delta)\frac{x-m_0}{\delta} + \delta\bigl(\frac{x-m_0}{\delta}\bigr)^2\bigr\} & \text{for } x \in (m_0, m_0+\delta)\\ f_0(x) & \text{for } x \in [m_0+\delta, 1],\end{cases}$$

so that $f_\delta \in \mathcal{F}$ and $m_0 + \delta$ is the unique inflection point of f_δ (since $x \mapsto (x-m_0)^2$ is strictly convex). Then based on similar (and slightly simpler) calculations to those for Lemma 3.5.11, we can apply Le Cam's two point lemma as above to obtain the conclusion of Proposition 3.3.4 when $\alpha \in (0,1)$. □

3.5.4 Projections onto classes of S-shaped functions

The purpose of this section is to introduce the general projection framework that underpins our estimation methodology, and to study the continuity properties of this projection. This allows us to deduce not only the consistency guarantees for our estimator, as stated in Proposition 3.1.2, but also to ensure its robustness to model misspecification; see Proposition 3.5.16 below.

For a finite Borel measure ν on $[0,1]$, we say that $x \in \operatorname{supp}\nu$ is an *isolated point* of $\operatorname{supp}\nu$ if there exists an open neighbourhood U of x such that $U \cap \operatorname{supp}\nu = \{x\}$. Denote by $\operatorname{csupp}\nu := \operatorname{conv}(\operatorname{supp}\nu)$ the *convex support* of ν, which is the smallest closed, convex set C with $\nu(C^c) = 0$. For Lebesgue measurable functions $f, g\colon [0,1] \to \mathbb{R} \cup \{\pm\infty\}$, we write $f \sim_\nu g$ if $f = g$ ν-almost everywhere, and noting that $\sim_\nu$ defines an equivalence relation on the set of such measurable functions, we denote by $[f]_\nu$ the $\sim_\nu$ equivalence class of f.

For $q \in [1,\infty)$, we write $L^q(\nu) \equiv L^q([0,1],\nu)$ for the space of Lebesgue measurable functions $f\colon [0,1] \to \mathbb{R}\cup\{\pm\infty\}$ such that $\|f\|_{L^q(\nu)} := \bigl(\int_{[0,1]} |f|^q\,d\nu\bigr)^{1/q} < \infty$, and define $\mathcal{L}^q(\nu) \equiv \mathcal{L}^q([0,1],\nu) := \{[f]_\nu : f \in L^q(\nu)\}$. When $q = 2$, recall that the bilinear form $\langle\cdot\,,\cdot\rangle_{L^2(\nu)}$ on $L^2(\nu)$ defined by $\langle f, g\rangle_{L^2(\nu)} := \int_{[0,1]} fg\,d\nu$ induces a Hilbert space structure on $\mathcal{L}^2(\nu)$.

For a Borel set $A \subseteq [0,1]$ and a Lebesgue measurable function $f\colon [0,1] \to \mathbb{R}$, let $\|f\|_{L^\infty(A,\nu)} := \inf\{B \geq 0 : |f(x)| \leq B$ for ν-almost every $x \in A\}$, where we adopt the convention that $\inf\emptyset = \infty$. A function $f \in [0,1] \to \mathbb{R}$ is said to be *locally bounded* at $x \in [0,1]$ if there exists $\varepsilon > 0$ such that f is bounded on $(x-\varepsilon, x+\varepsilon) \cap [0,1]$.

The following proposition provides some basic structural properties of the classes $\mathcal{F}^m$. See Section 3.6.3 for the proofs of all results in this subsection.

Proposition 3.5.12. *If $m \in [0,1]$ and ν is a Borel probability measure on $[0,1]$, then $\mathcal{F}_\nu^m := \{[f]_\nu : f \in \mathcal{F}^m\}$ is a convex cone in $\mathcal{L}^2(\nu)$. Moreover, the following hold for all $m \in [0,1]$:*

(a) $\{[f]_\nu : f \in \mathcal{F}^m$ is Lipschitz$\}$ is dense in $\mathcal{F}_\nu^m$ (with respect to the topology induced by $\|\cdot\|_{L^2(\nu)}$).

(b) Let $\tilde{m} := \operatorname{argmin}_{x\in\operatorname{csupp}\nu}|x - m|$. Then $\mathcal{F}_\nu^m$ is a dense subset of $\mathcal{F}_\nu^{\tilde{m}}$.

(c) *$\mathcal{F}^m_\nu$ is closed in $\mathcal{L}^2(\nu)$ if and only if at least one of the following conditions is satisfied:*

   (i) *$\nu([0,m]) > 0$ and $\nu([m,1]) > 0$;*

   (ii) *$\max(\operatorname{supp}\nu) < m$ and $\max(\operatorname{supp}\nu)$ is an isolated point of $\operatorname{supp}\nu$;*

   (iii) *$\min(\operatorname{supp}\nu) > m$ and $\min(\operatorname{supp}\nu)$ is an isolated point of $\operatorname{supp}\nu$.*

(d) *Suppose that none of the conditions (i)–(iii) hold, and let E_ν be the interval containing all $x \in (\min(\operatorname{supp}\nu), \max(\operatorname{supp}\nu))$ as well as those $x \in \{\min(\operatorname{supp}\nu), \max(\operatorname{supp}\nu)\}$ for which $\nu(\{x\}) > 0$. Denote by $\operatorname{Cl}\mathcal{F}^m_\nu$ the closure of $\mathcal{F}^m_\nu$ in $\mathcal{L}^2(\nu)$. Then*

$$\operatorname{Cl}\mathcal{F}^m_\nu = \begin{cases} \{[f]_\nu : f \in L^2(\nu) \text{ and } f|_{E_\nu} \text{ is convex and increasing}\} & \text{if } \max(\operatorname{supp}\nu) \le m \\ \{[f]_\nu : f \in L^2(\nu) \text{ and } f|_{E_\nu} \text{ is concave and increasing}\} & \text{if } \min(\operatorname{supp}\nu) \ge m. \end{cases}$$

For example, if ν is Lebesgue measure on $[0,1]$, then $\mathcal{F}^m_\nu$ is a closed subset of $\mathcal{L}^2(\nu)$ if and only if $m \in (0,1)$.

Let $\mathcal{P}$ be the class of probability distributions P on $[0,1]\times\mathbb{R}$ such that $\int_{[0,1]\times\mathbb{R}} y^2\,dP(x,y) < \infty$. For $P \in \mathcal{P}$, denote by P^X the marginal distribution on $[0,1]$ induced by the coordinate projection $(x,y) \mapsto x$, and for $f \in L^2(P^X)$, define

$$L(f,P) := \int_{[0,1]\times\mathbb{R}} \bigl(y - f(x)\bigr)^2\,dP(x,y). \tag{3.5.37}$$

Introducing $(X,Y) \sim P$, we say that $f_P\colon [0,1] \to \mathbb{R}$ is a *regression function for P* if $f_P(X)$ is a version of $\mathbb{E}(Y|\,X)$. Then $f_P \in L^2(P^X)$ and

$$\begin{aligned} L(f,P) = \mathbb{E}\bigl(\{Y - f(X)\}^2\bigr) &= \mathbb{E}\bigl(\{Y - f_P(X)\}^2\bigr) + \mathbb{E}\bigl(\{f_P(X) - f(X)\}^2\bigr) \\ &= \mathbb{E}\bigl(\{Y - f_P(X)\}^2\bigr) + \|f_P - f\|^2_{L^2(P^X)} \end{aligned} \tag{3.5.38}$$

for all $f \in L^2(P^X)$. Note that by (3.5.38), we have $L(f_n,P) \to L(f,P)$ whenever $\|f_n - f\|_{L^2(P^X)} \to 0$. Thus, for each $m \in [0,1]$, it follows from Proposition 3.5.12(a) that $L^*_m(P) := \inf_{f\in\mathcal{F}^m} L(f,P)$ is the infimum of $f \mapsto L(f,P)$ over all Lipschitz $f \in \mathcal{F}^m$.

For $\delta \ge 0$, let $\psi^\delta_m(P) := \{f \in \mathcal{F}^m : L(f,P) \le L^*_m(P) + \delta\}$, which is a non-empty set when $\delta > 0$. In Corollary 3.5.13(d) below, we give sufficient conditions for $\psi^0_m(P)$ to be non-empty, i.e. for $f \mapsto L(f,P)$ to attain its infimum $L^*_m(P)$ over $\mathcal{F}^m$.

Recall that if E is a closed, convex subset of a Hilbert space $(H, \|\cdot\|)$, then for each $x \in H$, there is a unique $y \in E$ such that $\|x - y\| = \min_{w\in E}\|x - w\|$, namely the *projection* of x onto E (e.g. Rudin, 1987, Theorem 4.10). In view of this and Proposition 3.5.12, we can now define projection maps $\psi^*_m\colon \mathcal{P} \to \mathcal{L}^2(P^X)$ associated with the convex function classes $\mathcal{F}^m$.

Corollary 3.5.13. *Fix $P \in \mathcal{P}$ and denote by P^X the corresponding marginal distribution on $[0,1]$. For each $m \in [0,1]$, let $\psi^*_m(P)$ be the collection of all $f\colon [0,1] \to \mathbb{R}$ such that $[f]_{P^X} \in \operatorname{Cl}\mathcal{F}^m_{P^X} \subseteq \mathcal{L}^2(P^X)$ and $L(f,P) = L^*_m(P)$. Then the following hold for all $m \in [0,1]$:*

(a) *$\psi^*_m(P)$ is a non-empty $\sim_{P^X}$ equivalence class containing $\psi^0_m(P)$.*

(b) *$\psi^*_m(P) \in \mathcal{L}^2(P^X)$, and if $\psi^0_m(P) \ne \emptyset$, then $\psi^*_m(P) \in \mathcal{L}^q(P^X)$ for all $q \in [1,\infty)$.*

(c) *Defining $\tilde m = \operatorname{argmin}_{x\in\operatorname{csupp}P^X}|x - m|$ as in Proposition 3.5.12(b), we have $\psi^*_m(P) = \psi^*_{\tilde m}(P)$ and $L^*_m(P) = L^*_{\tilde m}(P)$. If $\psi^0_m(P)$ is non-empty, then so is $\psi^0_{\tilde m}(P)$.*

(d) *$\psi^0_m(P) = \psi^*_m(P) \cap \mathcal{F}^m$ is non-empty if at least one of the following holds:*

(i) *$\mathcal{F}^m_{P^X}$ is a closed subset of $\mathcal{L}^2(P^X)$, i.e. if m, P^X satisfy at least one of the conditions (i)–(iii) in Proposition 3.5.12(c);*

(ii) *$m = \tilde{m}$ and P has a regression function f_P that is locally bounded at $\tilde{m}$.*

(e) *All functions in $\psi^0_m(P)$ agree on $(\operatorname{supp} P^X) \setminus \{m\}$. If in addition $P^X(\{m\}) > 0$ or all elements of $\psi^0_m(P)$ are continuous (at m), then they all agree on $\operatorname{supp} P^X$.*

(f) *When $m \in \operatorname{supp} P^X$ and $P^X(\{m\}) = 0$, all elements of $\psi^0_m(P)$ agree on $\operatorname{supp} P^X$ if and only if all elements of $\psi^0_m(P)$ are continuous (at m).*

(g) *Suppose that at least one element of $\psi^0_m(P)$ is continuous (at m), and moreover that $\operatorname{supp} P^X$ has non-empty intersection with both $(m-\varepsilon, m)$ and $(m, m+\varepsilon)$ for all $\varepsilon > 0$. Then all elements of $\psi^0_m(P)$ are continuous (at m) and agree on $\operatorname{supp} P^X$.*

Remark. If $m \in \operatorname{Int}(\operatorname{csupp} P^X)$, then m, P^X satisfy condition (i) in Proposition 3.5.12(c), so $\psi^0_m(P) \neq \emptyset$ in this case by (d) above. Moreover, in condition (ii) in part (d), we need only insist that f_P is bounded on $\operatorname{Int}(\operatorname{csupp} P^X) \cap (\tilde{m} - \varepsilon, \tilde{m} + \varepsilon)$ for some $\varepsilon > 0$; indeed, setting $\tilde{z} := \operatorname{argmin}_{x \in \operatorname{csupp} P^X} |z - x|$ for $z \in [0,1]$, we can instead work with $\tilde{f}_P \colon z \mapsto f_P(\tilde{z})$, which is another regression function for P that is bounded on $(\tilde{m} - \varepsilon, \tilde{m} + \varepsilon)$. As for (e, f, g), recall that all elements of $\mathcal{F}^m$ are continuous on $[0,1] \setminus \{m\}$, so being continuous on $[0,1]$ is equivalent to being continuous at m for all such functions.

Next, we investigate the continuity of the maps $(m, P) \mapsto L^*_m(P)$ and $(m, P) \mapsto \psi^*_m(P)$ with respect to a suitable topology on $[0,1] \times \mathcal{P}$. Recall that for $q \in [1, \infty)$ and $d \in \mathbb{N}$, the *q-Wasserstein distance* between probability measures P_1, P_2 on $\mathbb{R}^d$ is defined by $W_q(P_1, P_2) := \inf_{(X,Y)} \mathbb{E}(\|X - Y\|^q)^{1/q}$, where the infimum is taken over all pairs of random variables X, Y defined on a common probability space with $X \sim P_1$ and $Y \sim P_2$. It is a standard fact that $W_q(P_n, P) \to 0$ if and only if $P_n \xrightarrow{d} P$ and $\int_{\mathbb{R}^d} \|w\|^q \, dP_n(w) \to \int_{\mathbb{R}^d} \|w\|^q \, dP(w)$.

In the result below, we equip $[0,1] \times \mathcal{P}$ with the product topology induced by the Euclidean metric on $[0,1]$ and the W_2 metric on $\mathcal{P}$.

Proposition 3.5.14. *Let $(m_n)_{n=1}^\infty$ be a sequence in $[0,1]$ that converges to some $m_0 \in [0,1]$. Fix $P \in \mathcal{P}$ and the corresponding marginal distribution P^X on $[0,1]$. Define $\tilde{m}_0 := \operatorname{argmin}_{x \in \operatorname{csupp} P^X} |x - m_0|$. Let $(P_n)_{n=1}^\infty$ be any sequence of probability measures in $\mathcal{P}$ such that $W_2(P_n, P) \to 0$. Then*

(a) *$\limsup_{n\to\infty} L^*_{m_n}(P_n) \leq L^*_{m_0}(P)$;*

(b) *$\liminf_{n\to\infty} L^*_{m_n}(P_n) \geq L^*_{m_0}(P)$ provided that $P^X(\{\tilde{m}_0\}) = 0$;*

(c) *$\lim_{n\to\infty} L^*_{m_n}(P) = L^*_{m_0}(P)$.*

Thus, for all $Q \in \mathcal{P}$, the map $m \mapsto L^*_m(Q)$ is continuous on $[0,1]$ and $L^*(Q) := \min_{m \in [0,1]} L^*_m(Q)$ is well-defined. Moreover,

(d) *$\sup_{m \in [0,1]} |L^*_m(P_n) - L^*_m(P)| \to 0$ and $L^*(P_n) \to L^*(P)$ as $n \to \infty$ provided that $P^X(\{m\}) = 0$ for all $m \in [0,1]$.*

For $\delta \geq 0$ and $Q \in \mathcal{P}$, define $\mathcal{I}^\delta(Q) := \{m \in [0,1] : L^*_m(Q) \leq L^*(Q) + \delta\}$ and $\mathcal{I}^*(Q) := \mathcal{I}^0(Q) = \operatorname{argmin}_{m \in [0,1]} L^*_m(Q)$. Let (δ_n) be any deterministic, non-negative sequence such that $\delta_n \to 0$. Then

(e) *$\sup_{m'_n \in \mathcal{I}^{\delta_n}(P_n)} \inf_{m^* \in \mathcal{I}^*(P)} |m'_n - m^*| \to 0$ as $n \to \infty$ provided that $P^X(\{m\}) = 0$ for all $m \in [0,1]$.*

If $P^X(\{\tilde{m}_0\}) = 0$, then the following hold as $n \to \infty$:

(f) $\sup_{f_n \in \psi^{\delta_n}_{m_n}(P_n)} \sup_{f^* \in \psi^*_{\tilde{m}_0}(P)} \|f_n - f^*\|_{L^\infty(A,P^X)} \to 0$ *for all closed sets* $A \subseteq (\operatorname{supp} P^X) \setminus \{\tilde{m}_0\}$*;*

(g) *If* $\psi^0_{\tilde{m}_0}(P) \neq \emptyset$*, then* $\sup_{f_n \in \psi^{\delta_n}_{m_n}(P_n)} \sup_{f^* \in \psi^0_{\tilde{m}_0}(P)} \sup_{x \in A} |f_n(x) - f^*(x)| \to 0$ *for all closed sets* $A \subseteq (\operatorname{supp} P^X) \setminus \{\tilde{m}_0\}$*.*

Suppose further that $m_0 \in \operatorname{Int}(\operatorname{csupp} P^X)$ *and* $P^X(\{m_0\}) = 0$*. Then* $\psi^0_{m_0}(P) \neq \emptyset$ *and the following hold as* $n \to \infty$*:*

(h) $\sup_{f_n \in \psi^{\delta_n}_{m_n}(P_n)} \sup_{f^* \in \psi^*_{m_0}(P)} \|f_n - f^*\|_{L^q(P^X)} \to 0$ *for all* $q \in [1, \infty)$*;*

(i) $\sup_{f_n \in \psi^{\delta_n}_{m_n}(P_n)} \sup_{f^* \in \psi^0_{m_0}(P)} \sup_{x \in \operatorname{supp} P^X} |(f_n - f^*)(x)| \to 0$ *provided that all elements of* $\psi^0_{m_0}(P)$ *agree on* $\operatorname{supp} P^X$*.*

Remark. Since $[0,1]$ is compact, the conclusion of (e) is equivalent to the following: for any sequence (m_n') with $m_n' \in \mathcal{I}^{\delta_n}(P_n)$ for all n, every subsequence of (m_n') has a further subsequence that converges to an element of $\mathcal{I}^*(P)$. When $m_0 \notin \operatorname{supp} P^X$, the conclusion of (i) is implied by (g). If instead $m_0 \in \operatorname{supp} P^X$, then by Corollary 3.5.13(f), the condition in (i) is satisfied if and only if all elements of $\psi^0_{m_0}(P)$ are continuous, and Corollary 3.5.13(g) provides a sufficient criterion for this.

Recall that $\mathcal{F} = \bigcup_{m \in [0,1]} \mathcal{F}^m$ denotes the set of S-shaped functions on $[0,1]$. For $P \in \mathcal{P}$ and $\delta \geq 0$, define $\psi^\delta(P) := \{f \in \mathcal{F} : L(f, P) \leq L^*(P) + \delta\}$, which is non-empty when $\delta > 0$, and note that $\psi^\delta(P) \subseteq \bigcup_{m \in \mathcal{I}^\delta(P)} \psi^\delta_m(P)$. Also, let $\psi^*(P) := \bigcup_{m \in \mathcal{I}^*(P)} \psi^*_m(P) \supseteq \bigcup_{m \in \mathcal{I}^*(P)} \psi^0_m(P) = \psi^0(P)$.

Corollary 3.5.15. *Fix* $P \in \mathcal{P}$ *and the corresponding marginal distribution* P^X *on* $[0,1]$*. Then*

(a) $\psi^0(P) \neq \emptyset$ *if and only if* $\psi^0_m(P) \neq \emptyset$ *for some* $m \in \mathcal{I}^*(P) \cap \operatorname{csupp} P^X$*, which is guaranteed if at least one of the following holds:*

  (i) $\mathcal{I}^*(P) \cap \operatorname{Int}(\operatorname{csupp} P^X) \neq \emptyset$*;*

  (ii) P *has a regression function that is locally bounded at each* $m \in \mathcal{I}^*(P) \cap \{\min(\operatorname{csupp} P^X), \max(\operatorname{csupp} P^X)\}$ *for which* $P^X(\{m\}) = 0$*.*

  If (ii) holds, then $\psi^0_m(P) \neq \emptyset$ *for all* $m \in \mathcal{I}^*(P) \cap \operatorname{csupp} P^X$*.*

Suppose that $P^X(\{m\}) = 0$ *for all* $m \in [0,1]$*. Let* $(P_n)_{n=1}^\infty$ *be a sequence in* $\mathcal{P}$ *such that* $W_2(P_n, P) \to 0$ *and let* (δ_n) *be any deterministic, non-negative sequence such that* $\delta_n \to 0$*. Then the following hold as* $n \to \infty$*:*

(b) $\sup_{f_n \in \psi^{\delta_n}(P_n)} \inf_{f^* \in \psi^*(P)} \|f_n - f^*\|_{L^\infty(A,P^X)} \to 0$ *for all closed sets* $A \subseteq (\operatorname{supp} P^X) \setminus \mathcal{I}^*(P)$*.*

(c) *Assume that* $\psi^0_m(P) \neq \emptyset$ *for all* $m \in \mathcal{I}^*(P) \cap \operatorname{csupp} P^X$ *and let* $\tilde{\mathcal{I}}^*(P)$ *be the set of* $m^* \in \mathcal{I}^*(P)$ *such that either* $m^* \notin \operatorname{Int}(\operatorname{csupp} P^X)$ *or not all elements of* $\psi^0_{m^*}(P)$ *are continuous. Then* $\sup_{f_n \in \psi^{\delta_n}(P_n)} \inf_{f^* \in \psi^0(P)} \sup_{x \in A} |(f_n - f^*)(x)| \to 0$ *for all closed sets* $A \subseteq (\operatorname{supp} P^X) \setminus \tilde{\mathcal{I}}^*(P)$*.*

(d) *If* $\mathcal{I}^*(P) \subseteq \operatorname{Int}(\operatorname{csupp} P^X)$*, then* $\sup_{f_n \in \psi^{\delta_n}(P_n)} \inf_{f^* \in \psi^0(P)} \|f_n - f^*\|_{L^q(P^X)} \to 0$ *for all* $q \in [1, \infty)$*.*

Remark. In (c), recall from Corollary 3.5.13(d) that $\psi^0_m(P) \neq \emptyset$ for all $m \in \operatorname{Int}(\operatorname{csupp} P^X)$, so we are assuming in addition here that $\psi^0_m(P) \neq \emptyset$ for all $m \in \mathcal{I}^*(P) \cap \{\min(\operatorname{csupp} P^X), \max(\operatorname{csupp} P^X)\}$, for which condition (ii) in (a) is a sufficient criterion.

In assertions (b)–(d), we see that $\psi^*(P)$ or $\psi^0(P)$ can be regarded as a 'limiting set' $\mathcal{M}$ to which the sets $\mathcal{M}_n = \psi^{\delta_n}(P_n)$ converge, in the sense that $\sup_{f_n \in \mathcal{M}_n} \inf_{f \in \mathcal{M}} \rho(f_n, f) \to 0$ for each of three different pseudometrics ρ. In the proof, we establish a slightly stronger conclusion for each ρ: for any sequence (f_n) with $f_n \in \mathcal{M}_n$ for all n, every subsequence of (f_n) has a further subsequence that converges to an element of $\mathcal{M}$ with respect to ρ. Note that unlike in Proposition 3.5.14(f)–(i), we take an infimum rather than a supremum over $\mathcal{M}$ in the convergence statements above. This is because we do not in general have $\rho(f,g) = 0$ for all $f,g \in \mathcal{M}$ (in contrast to the sets $\psi_m^*(P)$ for each fixed $m \in [0,1]$). See Example 3.4 below in Section 3.6.4, where we also demonstrate through Examples 3.2 and 3.3 that if certain technical conditions in Proposition 3.5.14 and Corollary 3.5.15 are dropped, then some of the conclusions fail to hold in general.

For a regression function $f_0 \colon [0,1] \to \mathbb{R}$ (that need not be S-shaped) and a sequence of models (3.1.1) indexed by $n \in \mathbb{N}$, we can now establish asymptotic convergence results for S-shaped LSEs and their inflection points, including under model misspecification. To this end, we apply the continuity results from the general projection theory above (specifically Proposition 3.5.14 and Corollary 3.5.15) to the empirical distributions $\mathbb{P}_n$.

Proposition 3.5.16. *Suppose that the following conditions hold:*

- *(i)* $(\mathbb{P}_n^X)$ *converges weakly to a distribution* P_0^X *on* $[0,1]$ *satisfying* $P_0^X(\{m\}) = 0$ *for all* $m \in [0,1]$*;*
- *(ii) For some distribution* P_ξ *with mean 0 and finite variance, we have* $\xi_{n1},\dots,\xi_{nn} \overset{\text{iid}}{\sim} P_\xi$ *for each* n*;*
- *(iii)* f_0 *is bounded on* $[0,1]$ *and continuous* P_0^X*-almost everywhere (i.e. the set of discontinuities of* f_0 *has* P_0^X *measure 0).*

Let $P_0 \in \mathcal{P}$ *be the distribution of* $(X, f_0(X) + \xi)$*, where* $X \sim P_0^X$ *and* $\xi \sim P_\xi$ *are independent, and define* $L_m^*(P_0)$ *for* $m \in [0,1]$ *and* $L^*(P_0), \psi^0(P_0)$*,* $\mathcal{I}^*(P_0)$*,* $\tilde{\mathcal{I}}^*(P_0)$ *as in Proposition 3.5.14 and Corollary 3.5.15. Then* $\psi^0(P_0) \neq \emptyset$*, and*

- *(a)* $\sup_{m\in[0,1]} |L_m^*(\mathbb{P}_n) - L_m^*(P_0)| \overset{p}{\to} 0$ *and* $L^*(\mathbb{P}_n) - L^*(P_0) \overset{p}{\to} 0$ *as* $n \to \infty$*, where* $L_m^*(\mathbb{P}_n) = S_n(\hat{f}_n^m)/n$ *and* $L^*(\mathbb{P}_n) = \min_{1\le j\le n} S_n(\hat{f}_n^{x_{nj}})/n$ *for* $m \in [0,1]$ *and* $n \in \mathbb{N}$*.*

For each n*, fix an LSE* $\tilde{f}_n$ *over* $\mathcal{F}$*, so that* $\tilde{f}_n \in \psi^0(\mathbb{P}_n)$*, and let* $\tilde{m}_n$ *be any inflection point of* $\tilde{f}_n$*. Then the following hold as* $n \to \infty$*:*

- *(b)* $\inf_{m^*\in\mathcal{I}^*(P_0)} |\tilde{m}_n - m^*| \overset{p}{\to} 0$*;*
- *(c)* $\inf_{f^*\in\psi^0(P_0)} \sup_{x\in A} |(\tilde{f}_n - f^*)(x)| \overset{p*}{\to} 0$ *for any closed set* $A \subseteq \operatorname{supp} P_0^X \setminus \tilde{\mathcal{I}}^*(P_0)$*;*
- *(d)* $\inf_{f^*\in\psi^0(P_0)} \|\tilde{f}_n - f^*\|_{L^q(P_0^X)} \overset{p*}{\to} 0$ *for all* $q \in [1,\infty)$*, provided that* $\mathcal{I}^*(P_0) \subseteq \operatorname{Int}(\operatorname{csupp} P_0^X)$*.*

Using the full strength of Proposition 3.5.14 and Corollary 3.5.15, we see that for a sequence of non-negative tolerances $\delta_n \to 0$, the conclusions above extend to sequences $(\tilde{f}_n)$ where each $\tilde{f}_n$ takes values in $\psi^{\delta_n}(\mathbb{P}_n)$, the set of approximate δ_n-minimisers of $f \mapsto S_n(f)$ over $\mathcal{F}$.

In the correctly specified setting where $f_0 \in \mathcal{F}^{m_0}$ for some unique $m_0 \in [0,1]$, Proposition 3.5.16 specialises to the consistency result stated as Proposition 3.1.2 in the main text.

3.6 Supplementary material

3.6.1 Proofs for Section 3.5.2

For reference, we state a result from convex analysis that generalises Lemmas 3.5.5 and 3.5.6.

Lemma 3.6.1. *Let* $\Lambda \subseteq \mathbb{R}^n$ *be a non-empty closed, convex set. For each* $y \in \mathbb{R}^n$*, there exists a unique projection of* y *onto* Λ*, given by* $\Pi_\Lambda(y) = \operatorname{argmin}_{u\in\Lambda} \|u - y\|$*, and we have the following:*

- *(a)* $\Pi_\Lambda(y)$ *is the unique* $\hat{y} \in \Lambda$ *for which* $\langle u - \hat{y}, y - \hat{y}\rangle \le 0$ *for all* $u \in \Lambda$*.*

(b) For each $u \in \Lambda$, we have $\Pi_\Lambda^{-1}(\{u\}) = u + N_\Lambda(u)$, where $N_\Lambda(u) := \{v \in \mathbb{R}^n \setminus \{0\} : \langle v, \tilde{u}\rangle \leq \langle v, u\rangle$ for all $\tilde{u} \in \Lambda\} \cup \{0\}$ is the normal cone *of Λ at u.*

Furthermore, each element of Λ is contained in the relative interior of a unique face of Λ. For each face $F \subseteq \Lambda$, we have the following:

(c) There is a closed convex cone $N_\Lambda(F)$ such that $N_\Lambda(u) = N_\Lambda(F)$ for all $u \in \operatorname{relint} F$, and $\Pi_\Lambda^{-1}(\operatorname{relint} F) = (\operatorname{relint} F) + N_\Lambda(F)$. If $u \in \operatorname{relint} F$ and $v \in N_\Lambda(F)$, then $\Pi_\Lambda(u+v) = u$.

(d) For all $y \in \Pi_\Lambda^{-1}(\operatorname{relint} F)$, we have $\Pi_\Lambda(y) = \Pi_{\operatorname{aff}(F)}(y)$, where $\operatorname{aff}(F)$ denotes the affine hull of F, i.e. the smallest affine subspace containing F.

(e) If in addition Λ is a finitely generated cone, then F and $N_\Lambda(F)$ are also finitely generated cones, and $\operatorname{span}(F)$ and $\operatorname{span}\big(N_\Lambda(F)\big)$ are complementary orthogonal subspaces. Thus, $\Pi_\Lambda^{-1}(\operatorname{relint} F) = (\operatorname{relint} F) + N_\Lambda(F)$ is an n-dimensional convex cone (with non-empty interior).

Proof. For (a, b) and the first assertion in (c), see Schneider (2014, Section 1.2), and (2.3) and Lemma 2.2.2 in Schneider (2014, Section 2.2). Using these, we now complete the proofs of (c, d, e).

(c) By the definition of $N_\Lambda(F)$, we have $\langle v, \tilde{u} - u\rangle \leq 0$ for all $v \in N_\Lambda(F)$, $\tilde{u} \in \operatorname{relint} F$ and $u \in \Lambda$, with equality when $u \in \operatorname{relint} F$. It now follows from (a) that $\Pi_\Lambda(u+v) = u$ for all $u \in \operatorname{relint} F$ and $v \in N_\Lambda(F)$.

(d) Take any $u \in \operatorname{aff}(F)$. Since $\Pi_\Lambda(y) \in \operatorname{relint} F$, we have $\Pi_\Lambda(y) + \lambda u$ for some sufficiently small $\lambda > 0$, so $\langle \lambda u, y - \Pi_\Lambda(y)\rangle = 0$. Thus, $\Pi_\Lambda(y) \in \operatorname{aff}(F)$ and $\langle u, y - \Pi_\Lambda(y)\rangle = 0$ for all $u \in \operatorname{aff}(F)$, so indeed $\Pi_\Lambda(y) = \Pi_{\operatorname{aff}(F)}(y)$.

(e) For a finitely generated cone Λ, this follows from Theorem 2.4.9 and (2.25) in Schneider (2014, Section 2.2). □

By applying Lemma 3.5.5, we can give an alternative self-contained proof of Lemma 3.5.6 for the cone $\Lambda^j \subseteq \mathbb{R}^j$ of increasing convex sequences based on $x_1, \dots, x_j$, whose generators $\pm u^0, u^1, \dots, u^{j-1}$ are specified in the paragraph below (3.2.1). For $A \subseteq [j-1]$, recall from Remark 3.5.1 that we write $P_A \in \mathbb{R}^{j \times j}$ for the matrix that represents the orthogonal projection $\Pi_{\mathcal{L}_A}$ onto $\mathcal{L}_A = \operatorname{span}\{u^{\ell'} : \ell' \in A \cup \{0\}\}$, the subspace consisting of all $v \in \mathbb{R}^j$ whose knots lie in A.

Proof of Lemma 3.5.6. For each $\tilde{v} \in \{v', v''\}$, we have $\Pi_\Lambda(\tilde{v}) \in F_A \subseteq \operatorname{Im}(U_A)$, and Lemma 3.5.5 implies that $\langle u^\ell, \tilde{v} - \Pi_\Lambda(\tilde{v})\rangle = 0$ for all $\ell \in A \cup \{0\}$. This shows that $P_A(\tilde{v}) = \Pi_\Lambda(\tilde{v}) \in \operatorname{relint} F_A$ for $\tilde{v} \in \{v', v''\}$. Now fix $t \in [0,1]$ and $v := (1-t)v' + tv''$. Then $P_A(v) = (1-t)P_A(v') + tP_A(v'') = (1-t)\Pi_\Lambda(v') + t\Pi_\Lambda(v'') \in \operatorname{relint} F_A$ by the convexity of $\operatorname{relint} F_A$. In addition, by applying Lemma 3.5.5 to $\Pi_\Lambda(v'), \Pi_\Lambda(v'')$, we deduce that

$$\langle u^\ell, v - P_A(v)\rangle = (1-t)\langle u^\ell, v' - \Pi_\Lambda(v')\rangle + t\langle u^\ell, v'' - \Pi_\Lambda(v'')\rangle \leq 0$$

for all $0 \leq \ell \leq j-1$, with equality if $\ell \in A \cup \{0\}$ (in view of the definition of P_A). It follows from Lemma 3.5.5 that $\Pi_\Lambda(v) = P_A(v) \in \operatorname{relint} F_A$, as required. □

Proof of Lemma 3.5.7. For (iv), we know from (iii) that $\Pi_{\Lambda^j}\big(v(t)\big) = P_{A_r} v(t)$ for all $t \in [t_r, t_{r+1}]$ after an iteration of (II). By applying Lemma 3.5.6, we deduce that there exist $\eta > 0$ and $A' \subseteq [j-1]$ with $A' \neq A_r$ such that $\hat{v}(t) := \Pi_{\Lambda^j}\big(v(t)\big) = P_{A'} v(t) \in \Lambda^j \cap \mathcal{L}_{A'} = \{u \in \Lambda^j : A(u) \subseteq A'\}$ for all $t \in [t_{r+1}, t_{r+1} + \eta]$. Now in (IV), note that

- If $\ell \in A_r \setminus A_r^-$, then $\lambda_\ell\big(\hat{v}(t_{r+1})\big) = \beta_\ell(t_{r+1}) > 0$, so $\ell \in A\big(\hat{v}(t_{r+1})\big) \subseteq A'$;
- If $\ell \in A'$, then $\gamma_\ell(t_{r+1}) = \langle u^\ell, v(t_{r+1}) - \hat{v}(t_{r+1})\rangle = \langle u^\ell, (I - P_{A'})v(t_{r+1})\rangle = 0$, so $\ell \in \{1 \leq \ell' \leq j-1 : \gamma_{\ell'}(t_{r+1}) = 0\} = A_r \cup A_r^+$.

Thus, $A_r \setminus A_r^- \subseteq A' \subseteq A_r \cup A_r^+$, so in all cases, (IV) is guaranteed to find subsets $A^\pm \subseteq A_r^\pm$ such that when we take $A_{r+1} = (A_r \setminus A^-) \cup A^+$, the next iteration of (II) strictly increases t. In particular, this always happens in scenario (a) where $|A_r^- \cup A_r^+| = 1$, since we necessarily have $A' = (A_r \setminus A_r^-) \cup A_r^+ = A_{r+1}$ in this case.

For (v), recall again that for each $r \in \mathbb{N}_0$, we have $\Pi_{\Lambda^j}\bigl(v(t)\bigr) = P_{A_r}v(t) \equiv \hat{v}_r(t)$ for all $t \in [t_r, t_{r+1}]$. As noted in (II), $\lambda_\ell\bigl(\hat{v}_r(t)\bigr)$ and $\langle u^\ell, v(t) - \hat{v}_r(t)\rangle$ vary linearly with t for all $\ell \in [j-1]$, so it follows from this and (3.5.11) that

$$t_{r+1} = \sup\bigl\{t \geq t_r : \lambda_\ell\bigl(\hat{v}_r(t)\bigr) \geq 0,\ \langle u^\ell, v(t) - \hat{v}_r(t)\rangle \leq 0 \text{ for all } 1 \leq \ell \leq j-1\bigr\}.$$

Thus, by Lemma 3.5.5, we cannot have $\hat{v}_r(t) = \Pi_{\Lambda^j}\bigl(v(t)\bigr)$ for any $t > t_{r+1}$, so $A_r \neq A_{r'}$ for all $r' > r$, as claimed. □

Degeneracies in Algorithm 2: It can be verified that there is a set $A \subseteq \mathbb{R}^j \times \mathbb{R}^j$ of Lebesgue measure 0 such that if $(v(0), v(1)) \notin A$, then no degeneracies occur on the trajectory of the algorithm. Thus, degeneracies are rarely an issue when $v(0), v(1)$ are obtained from simulated or real data rather than artificially constructed (see Example 3.1). To avoid them in practice, Fraser and Massam (1989, page 73) and Meyer (1999, page 28) suggest slightly perturbing $v(0), v(1)$ or some intermediate $v(t_r)$. The approach we outline in Stage (IV) covers all eventualities in the degenerate scenario (b), but this can be time-consuming when $|A_r^- \cup A_r^+|$ is large.

In the special case where $u = v(0) - v(1)$ is a positive multiple of $u^{j-1} = e_j = (0, \ldots, 0, 1) \in \mathbb{R}^j$ (which is of particular relevance in the `SeqConReg` procedure in Section 3.2), a more efficient alternative to (IV) is as follows:

(IV') Instead define $A_r^- := \{\ell \in A_r : \beta_\ell(t_{r+1}) = 0,\ \hat{\lambda}_\ell^{A_r}(u) > 0\}$ and $A_r^+ := \{\ell \in A_r^c : \gamma_\ell(t_{r+1}) = 0,\ \hat{\zeta}_\ell^{A_r}(u) < 0\}$, and let $\ell_{\max} := \max(A_r^- \cup A_r^+)$. Let $A_{r+1} := A_r \setminus \{\ell_{\max}\}$ if $\ell_{\max} \in A_r^-$ and otherwise let $A_{r+1} := A_r \cup \{\ell_{\max}\}$ if $\ell_{\max} \in A_r^+$. Then execute (II) and (III) with this A_{r+1} (and $r+1$ in place of r throughout).

If there is a degeneracy at t_{r+1}, then when we run this modified algorithm, there may be several subsequent iterations of (II) in which t does not increase (i.e. we remain at t_{r+1}). Nevertheless, the choice of $\ell_{\max} = \max(A_r^- \cup A_r^+)$ in (IV') ensures that property (iv) still holds, and hence that the algorithm terminates with the exact solution (usually after fewer iterations than in the original).

Proposition 3.6.2. *Suppose that $u = v(0) - v(1)$ is a positive multiple of $u^{j-1} = e_j \in \mathbb{R}^j$. Then with modification (IV'), Algorithm 2 terminates with the correct solution after finitely many steps, and the following hold for any $r \in \mathbb{N}_0$:*

(a) $\max A_r \geq \max A_{r+1}$; in other words, if $\max A_r < \ell \leq j-1$, then $\ell \notin A_{r'}$ for any $r' > r$.

(b) Let $\ell_r := \max(\{\ell \in A_r : \ell + 1 \in A_r\} \cup \{0\})$. Then in (3.5.12), we have $\hat{\lambda}_\ell^{A_r}(u) \equiv \lambda_\ell(P_{A_r}u) = 0$ for all $0 \leq \ell \leq \ell_r - 1$ and $\hat{\zeta}_\ell^{A_r}(u) \equiv \langle u^\ell, (I - P_{A_r})u\rangle = 0$ for all $0 \leq \ell \leq \ell_r + 1$.

This follows from Lemma 3.6.3 below, which captures some specific structural features of the generators $\pm u^0, u^1, \ldots, u^{j-1}$ of Λ^j. The facts in (a) and (b) lead to some additional computational shortcuts in Algorithm 2 when u is a positive multiple of e_j. Specifically, when computing t_{r+1} in Stage (II) of the procedure, it follows from Proposition 3.6.2 that we need only compute the ratios in (3.5.12) for $\ell_r < \ell \leq \max A_r$. Thus, when $t \geq t_r$, we can drop all $\beta_\ell(t)$ and $\gamma_\ell(t)$ with $\ell > \max A_r$, and when updating the primal and dual variables for use in subsequent iterations, no calculations are needed to see that $\beta_\ell(t_{r+1}) = \beta_\ell(t_r)$ and $\gamma_\ell(t_{r+1}) = \gamma_\ell(t_r)$ for all $1 \leq \ell \leq \ell_r$.

Example 3.1. We can actually write down explicitly the sequence of 'active sets' $A_0, A_1, \ldots$ obtained by Algorithm 2 in the special case where $v(0) \in \Lambda^j$ and $u = v(0) - v(1)$ is a positive multiple of

e_j. This can happen if for example in (3.2.2), the observations $Y_1, \ldots, Y_j$ are drawn according to a *noiseless* regression model (3.1.1) in which f_0 is increasing and convex on $[x_1, x_{j-1}]$. With $A_0 = A\big(v(0)\big)$, it turns out that for $r \in \mathbb{N}_0$, we have

$$A_{r+1} = \begin{cases} A_r \setminus \{\max A_r\} & \text{if } \max A_r - 1 \in A_r \text{ or } \max A_r = j-1 \\ A_r \cup \{\max A_r - 1\} & \text{if } \max A_r - 1 \notin A_r \text{ and } \max A_r < j-1. \end{cases} \tag{3.6.1}$$

Indeed, given that $v(0) \in \Lambda^j$ and hence that $\gamma_\ell(0) = 0$ for all $0 \leq \ell \leq j-1$, we can apply Proposition 3.6.2 to establish inductively that $\gamma_\ell(t_{r+1}) = 0$ for all $0 \leq \ell \leq \max A_r$ and $r \in \mathbb{N}_0$. In particular, we always have $A_r^+ = \{1, \ldots, \max A_r - 1\} \cap A_r^c$, and

- If $\max A_r - 1 \in A_r$ or $\max A_r = j-1$, then $t_r < t_{r+1}$ and $A_r^- = \{\max A_r\}$;
- If $\max A_r - 1 \notin A_r$ and $\max A_r < j-1$, then $t_r = t_{r+1}$ and $A_r^- = \emptyset$.

Note that unless $\{1, \ldots, \max A_r - 2\} \subseteq A_r$, there is a degeneracy at t_{r+1}, so we use (IV') above to form the next 'active set' A_{r+1}. In addition, we have $\max A_r > \max A_{r+2}$ for all $r \in \mathbb{N}_0$ in view of (3.6.1), so the number of distinct 'active sets' on the trajectory of Algorithm 2 is at most $2(j-1)$. This is much less than 2^{j-1}, the total number of subsets of $[j-1]$, and an open question is whether for general $v(0) \in \mathbb{R}^j$ (and $u = v(0) - v(1)$ as above), the number of 'active sets' is necessarily bounded above by a polynomial in j. If this is always true (or true in 'most' cases), then our sequential procedure for increasing convex regression is guaranteed to have a worst-case (or average-case) complexity that is at most polynomial in the number of observations n.

For fixed $j \in [n]$, $\ell \in [j-1]$ and $A \subseteq [j-1]$, Lemma 3.6.3 determines the signs of the entries of $(I - P_A)u^\ell \in \mathbb{R}^j$ indexed by $A \cup \{\ell\}$. This yields useful information on how the primal and dual variables change in Algorithm 2 when the vector $u = v(0) - v(1)$ therein is a positive multiple of e_j. This enables us to justify the more efficient implementation (IV') of Stage (IV) of this procedure, as well as assertions (a) and (b) in Proposition 3.6.2 on the composition of the resulting active sets.

We write $e_1, \ldots, e_j$ for the standard basis vectors in $\mathbb{R}^j$ and $\langle \cdot, \cdot \rangle$ for the standard Euclidean inner product. For $t \in \mathbb{R}$, let $\mathrm{sgn}(t) := (|t|/t)\mathbb{1}_{\{t \neq 0\}}$.

Lemma 3.6.3. *For $A \subseteq [j-1]$, enumerate the elements of A as $a_1 > a_2 > \cdots > a_m$, and let $a_0 = j$ and $a_{m+1} = 0$. Fix $\ell \in [j-1]$. Then $(I - P_A)u^\ell \in \mathcal{L}_{A \cup \{\ell\}}$, and $(I - P_A)u^\ell = 0$ if and only if $\ell \in A$.*

Suppose now that $\ell \notin A$ and let $q \in [m+1]$ be such that $a_q < \ell < a_{q-1}$. Define $q_- := \max(\{1 \leq \tilde{q} \leq q-1 : a_{\tilde{q}-1} = a_{\tilde{q}} + 1\} \cup \{0\})$ and $q_+ := \min(\{q+1 \leq \tilde{q} \leq m : a_{\tilde{q}-1} = a_{\tilde{q}} + 1\} \cup \{m+1\})$. Then $\langle (I - P_A)u^\ell, e_\ell \rangle < 0$, $\langle P_A u^\ell, e_1 \rangle = \langle P_A u^\ell, e_{a_m} \rangle$, and for $0 \leq s \leq m$, we have

$$\mathrm{sgn}\big(\langle (I - P_A)u^\ell, e_{a_s} \rangle\big) = \begin{cases} (-1)^{s-q} & \text{if } q \leq s < q_+ \\ (-1)^{q-1-s} & \text{if } q_- \leq s \leq q-1 \\ 0 & \text{if } s < q_+ \text{ or } s \geq q_+. \end{cases} \tag{3.6.2}$$

Proof of Lemma 3.6.3. The generators $u^0, u^1, \ldots, u^{j-1}$ of the cone Λ^j are linearly independent, so $u^\ell \equiv (u_1^\ell, \ldots, u_j^\ell) = \big((x_i - x_\ell)^+ : 1 \leq i \leq j\big) \in \mathcal{L}_A$ (i.e. $(I - P_A)u^\ell = 0$) if and only if $\ell \in A$. Suppose henceforth that $\ell \notin A$ and let $\tilde{z} \equiv (\tilde{z}_1, \ldots, \tilde{z}_j) := P_A u^\ell = \mathrm{argmin}_{z \in \mathcal{L}_A} \|u^\ell - z\|$. Then $u^\ell - \tilde{z} = (I - P_A)u^\ell \in \mathrm{span}(\{u^\ell\} \cup \mathcal{L}_A) = \mathcal{L}_{A \cup \{\ell\}}$, so $u^\ell - \tilde{z}$ is determined by $\{u_i^\ell - \tilde{z}_i = \langle (I - P_A)u^\ell, e_i \rangle : i \in A \cup \{\ell\}\}$.

To establish (3.6.2), we make the following additional definitions. For $z \in \mathbb{R}^j$ and $J = \{b, b+1, \ldots, b'\}$ with $1 \leq b \leq b' \leq j$, we write $z_J = (z_b, z_{b+1}, \ldots, z_{b'})$ for the subvector of z indexed by J.

For $s \in [m]$, partition $[j]$ into the subsets

$$J_s^+ := \{1, \dots, a_s\}, \quad J_s := \{a_s + 1, \dots, a_{s-1} - 1\}, \quad J_s^- := \{a_{s-1}, \dots, j\},$$

and for $i \in J_s$, let $t_i^{J_s} := (x_i - x_{a_s})/(x_{a_{s-1}} - x_{a_s}) \in (0,1)$, so that any affine sequence based on $(x_i : i \in J_s)$ can be written in the form $v^{J_s}(\lambda, \vartheta) := \big((1 - t_i^{J_s})(u_{a_s}^{\ell} - \lambda) + t_i^{J_s}(u_{a_{s-1}}^{\ell} - \vartheta) : a_s + 1 \leq i \leq a_{s-1} - 1\big)$ for some $\lambda, \vartheta \in \mathbb{R}$. Moreover,

$$\mathcal{L}_{A,s}^+(\lambda) := \{z_{J_s^+} : z \in \mathcal{L}_A,\, z_{a_s} = \lambda\} \subseteq \mathbb{R}^{|J_s^+|} \text{ and } \mathcal{L}_{A,s}^-(\lambda) := \{z_{J_s^-} : z \in \mathcal{L}_A,\, z_{a_{s-1}} = \lambda\} \subseteq \mathbb{R}^{|J_s^-|}$$

are affine subspaces for each $\lambda \in \mathbb{R}$, and $\mathcal{L}_{A,s}^{\pm}(\lambda) = \lambda \mathcal{L}_{A,s}^{\pm}(1)$ if $\lambda \neq 0$, so $\tilde{v}^{J_s^{\pm}} := \operatorname{argmin}_{v \in \mathcal{L}_{A,s}^{\pm}(1)} \|v\|$ are well-defined and $\lambda \tilde{v}^{J_s^{\pm}} = \operatorname{argmin}_{v \in \mathcal{L}_{A,s}^{\pm}(\lambda)} \|v\|$ for all $\lambda \in \mathbb{R}$.

Claim 1. *Let $\star \in \{+,-\}$ and $s \in [m-1]$ be such that $a_s, a_{s\star1} \in J_q^\star$. If $|a_s - a_{s\star1}| = 1$, then $\tilde{v}_{a_{s\star1}}^{J_q^\star} = 0$. Otherwise, if $|a_s - a_{s\star1}| > 1$, then $\operatorname{sgn}\big(\tilde{v}_{a_{s\star1}}^{J_q^\star}\big) = -\operatorname{sgn}\big(\tilde{v}_{a_s}^{J_q^\star}\big)$. Thus,*

$$\operatorname{sgn}\big(\tilde{v}_{a_s}^{J_q^+}\big) = \begin{cases} (-1)^{s-q} & \text{if } q \leq s < q_+ \\ 0 & \text{if } q_+ \leq s \leq m; \end{cases} \quad \operatorname{sgn}\big(\tilde{v}_{a_s}^{J_q^-}\big) = \begin{cases} (-1)^{q-1-s} & \text{if } q_- \leq s \leq q-1 \\ 0 & \text{if } 0 \leq s < q_-. \end{cases}$$

Proof of Claim 1. We focus on the case $\star = +$; the arguments for $\star = -$ are similar. Note that $a_s, a_{s+1} \in J_s^+$ precisely when $q \leq s \leq m-1$. For any such s and $\mu \in \mathbb{R}$, define $\tilde{v}^{J_q^+}(s;\mu) \equiv \big(\tilde{v}_i^{J_q^+}(s,\mu) : 1 \leq i \leq a_q\big)$ by

$$\tilde{v}_i^{J_q^+}(s;\mu) := \begin{cases} \mu \tilde{v}_i^{J_{s+1}^+} = \operatorname{argmin}_{v \in \mathcal{L}_{A,s+1}^+(\mu)} \|v\| & \text{for } i \in J_{s+1}^+ = \{1, \dots, a_{s+1}\} \\ (1 - t_i^{J_{s+1}})\mu + t_i^{J_{s+1}} \tilde{v}_{a_s}^{J_q^+} = v_i^{J_{s+1}}\big(-\mu, -\tilde{v}_{a_s}^{J_q^+}\big) & \text{for } i \in J_{s+1} = \{a_{s+1} + 1, \dots, a_s - 1\} \\ \tilde{v}_i^{J_q^+} & \text{for } i \in J_{s+1}^- \cap J_q^+ = \{a_s, \dots, a_q\}. \end{cases}$$

Then $\tilde{v}_{a_s}^{J_q^+}(s;\mu) = \tilde{v}_{a_s}^{J_q^+}$, and since $\mu \tilde{v}^{J_{s+1}^+} \in \mathcal{L}_{A,s+1}^+(\mu)$, we have $\tilde{v}_{a_{s+1}}^{J_q^+}(s;\mu) = \mu$, so $\tilde{v}^{J_q^+}(s;\mu) \in \mathcal{L}_{A,q}^+(1)$. Observe in addition that $\tilde{v}^{J_q^+}\big(s; \tilde{v}_{a_{s+1}}^{J_q^+}\big) = \tilde{v}^{J_q^+}$; indeed, $\tilde{v}_i^{J_q^+}\big(s; \tilde{v}_{a_{s+1}}^{J_q^+}\big) = \tilde{v}_i^{J_q^+}$ for $a_{s+1} + 1 \leq i \leq a_q$ and

$$\begin{aligned} \tilde{\mathcal{L}}_{A,q,s+1}^+ &:= \big\{v \equiv (v_1, \dots, v_{a_q}) \in \mathcal{L}_{A,q}^+ : v_i = \tilde{v}_i^{J_q^+} \text{ for } a_{s+1} + 1 \leq i \leq a_q\big\} \\ &= \big\{(v_1, \dots, v_{a_q}) \in \mathbb{R}^{a_q} : v_{J_{s+1}^+} \in \mathcal{L}_{A,s+1}^+\big(\tilde{v}_{a_{s+1}}^{J_q^+}\big),\, v_i = \tilde{v}_i^{J_q^+} \text{ for } a_{s+1} + 1 \leq i \leq a_q\big\}, \end{aligned}$$

so $\tilde{v}^{J_q^+} = \operatorname{argmin}_{v \in \mathcal{L}_{A,q}^+(1)} \|v\| = \operatorname{argmin}_{v \in \tilde{\mathcal{L}}_{A,q,s+1}^+} \|v\|$ satisfies

$$(\tilde{v}^{J_q^+})_{J_{s+1}^+} = \operatorname*{argmin}_{v' \in \mathcal{L}_{A,s+1}^+\left(\tilde{v}_{a_{s+1}}^{J_q^+}\right)} \|v'\| = \tilde{v}_{a_{s+1}}^{J_q^+} \tilde{v}^{J_{s+1}^+} = \big(\tilde{v}^{J_q^+}(s; \tilde{v}_{a_{s+1}}^{J_q^+})\big)_{J_{s+1}^+}.$$

Thus,

$$\mu \mapsto r_s(\mu) := \|\tilde{v}^{J_q^+}(s;\mu)\|^2 = \mu^2 \|\tilde{v}^{J_{s+1}^+}\|^2 + \sum_{i \in J_{s+1}} \big((1 - t_i^{J_{s+1}})\mu + t_i^{J_{s+1}} \tilde{v}_{a_s}^{J_q^+}\big)^2 + \sum_{i=a_s}^{a_q} \big(\tilde{v}_i^{J_q^+}\big)^2$$

is a quadratic function with $r_s\big(\tilde{v}_{a_{s+1}}^{J_q^+}\big) = \|\tilde{v}^{J_q^+}\|^2 = \min_{v \in \mathcal{L}_{A,q}^+(1)} \|v\|^2 = \min_{\mu \in \mathbb{R}} r_s(\mu)$, so

$$0 = r_s'\big(\tilde{v}_{a_{s+1}}^{J_q^+}\big) = 2\tilde{v}_{a_{s+1}}^{J_q^+} \|\tilde{v}^{J_{s+1}^+}\|^2 + 2 \sum_{i \in J_{s+1}} \big((1 - t_i^{J_{s+1}})\tilde{v}_{a_{s+1}}^{J_q^+} + t_i^{J_{s+1}} \tilde{v}_{a_s}^{J_q^+}\big)\big(1 - t_i^{J_{s+1}}\big). \tag{3.6.3}$$

Now $\|\tilde{v}^{J^+_{s+1}}\|^2 > 0$ by the definition of $\tilde{v}^{J^+_{s+1}} \in \mathcal{L}^+_{A,s+1}(1)$, so if $a_s = a_{s+1}+1$, i.e. $J_{s+1} = \emptyset$, then $\tilde{v}^{J^+_q}_{a_{s+1}} = 0$ by (3.6.3). On the other hand, suppose instead that $a_s > a_{s+1}+1$, in which case $J_{s+1} \neq \emptyset$. If $\tilde{v}^{J^+_q}_{a_s} = 0$, then $\tilde{v}^{J^+_q}_{a_{s+1}} = 0$ by (3.6.3). When $\tilde{v}^{J^+_q}_{a_s} > 0$, we must have $\tilde{v}^{J^+_q}_{a_{s+1}} < 0$, since otherwise the first term on the right-hand side of (3.6.3) would be non-negative and each summand in the second term would be strictly positive, contradicting the fact that $r'_s\big(\tilde{v}^{J^+_q}_{a_{s+1}}\big) = 0$. Similarly, if $\tilde{v}^{J^+_q}_{a_s} < 0$, then $\tilde{v}^{J^+_q}_{a_{s+1}} > 0$. This completes the proof of the claim. □

Next, note that $u^\ell_{J^+_q} = 0 \in \mathcal{L}^+_{A,q}(0) = \mathcal{L}^+_{A,q}(u^\ell_{a_q})$ and $u^\ell_{J^-_q} = (x_i - x_\ell : a_{q-1} \leq i \leq j) \in \mathcal{L}^-_{A,q}(u^\ell_{a_{q-1}})$. Thus, for each $(\lambda, \vartheta) \in \mathbb{R}^2$, we have

$$\begin{aligned}\mathcal{L}^q_A(\lambda,\vartheta) &:= \{z \in \mathcal{L}_A : (u^\ell - z)_{a_q} = \lambda,\ (u^\ell - z)_{a_{q-1}} = \vartheta\} \\ &= \big\{z \in \mathcal{L}_A : (u^\ell - z)_{J^+_q} \in \mathcal{L}^+_{A,q}(\lambda),\ (u^\ell - z)_{J^-_q} \in \mathcal{L}^-_{A,q}(\vartheta),\ z_{J_q} = v^{J_q}(\lambda,\vartheta)\big\},\end{aligned} \tag{3.6.4}$$

and the unique minimiser $\tilde{z}(\lambda,\vartheta)$ of $z \mapsto \|u^\ell - z\|^2 = \|(u^\ell - z)_{J^+_q}\|^2 + \|(u^\ell - z)_{J_q}\|^2 + \|(u^\ell - z)_{J^-_q}\|^2$ over $\mathcal{L}^q_A(\lambda,\vartheta)$ satisfies $\tilde{z}(\lambda,\vartheta)_{J_q} = v^{J_q}(\lambda,\vartheta)$, $\big(u^\ell - \tilde{z}(\lambda,\vartheta)\big)_{J^+_q} = \mathrm{argmin}_{v \in \mathcal{L}^+_{A,q}(\lambda)} \|v\| = \lambda \tilde{v}^{J^+_q}$ and $\big(u^\ell - \tilde{z}(\lambda,\vartheta)\big)_{J^-_q} = \mathrm{argmin}_{v \in \mathcal{L}^-_{A,q}(\vartheta)} \|v\| = \vartheta \tilde{v}^{J^-_q}$. Let

$$\begin{aligned} r(\lambda,\vartheta) &:= \min_{z \in \mathcal{L}^q_A(\lambda,\vartheta)} \|u^\ell - z\|^2 = \|u^\ell - \tilde{z}(\lambda,\vartheta)\|^2 = \|\lambda\tilde{v}^{J^+_q}\|^2 + \|u^\ell_{J_q} - v^{J_q}(\lambda,\vartheta)\|^2 + \|\vartheta\tilde{v}^{J^-_q}\|^2 \\ &= \lambda^2\,\|\tilde{v}^{J^+_q}\|^2 + \sum_{i \in J_q}\big(u^\ell_i - (1 - t^{J_q}_i)(u^\ell_{a_q} - \lambda) - t^{J_q}_i(u^\ell_{a_{q-1}} - \vartheta)\big)^2 + \vartheta^2\,\|\tilde{v}^{J^-_q}\|^2,\end{aligned}$$

so that $(\lambda,\vartheta) \mapsto r(\lambda,\vartheta)$ is a quadratic form with

$$\nabla r(\lambda,\vartheta) = 2\lambda\,\|\tilde{v}^{J^+_q}\|^2 \begin{pmatrix}1\\0\end{pmatrix} + 2\sum_{i \in J_q}\big(u^\ell_i - v^{J_q}_i(\lambda,\vartheta)\big)\begin{pmatrix}1 - t^{J_q}_i\\ t^{J_q}_i\end{pmatrix} + 2\vartheta\,\|\tilde{v}^{J^-_q}\|^2\begin{pmatrix}0\\1\end{pmatrix} \tag{3.6.5}$$

for each $(\lambda,\vartheta) \in \mathbb{R}^2$, and $\tilde{z} = P_A u^\ell$ satisfies $\|u^\ell - \tilde{z}\|^2 = \min_{z \in \mathcal{L}_A}\|u^\ell - z\|^2 = \min_{(\lambda,\vartheta)\in\mathbb{R}^2} r(\lambda,\vartheta)$. Thus, writing $\tilde{\lambda} := (u^\ell - \tilde{z})_{a_q} = \langle (I - P_A)u^\ell, e_{a_q}\rangle$ and $\tilde{\vartheta} := (u^\ell - \tilde{z})_{a_{q-1}} = \langle (I - P_A)u^\ell, e_{a_{q-1}}\rangle$, we have $\tilde{z} = \tilde{z}(\tilde{\lambda},\tilde{\vartheta})$ and $(\tilde{\lambda},\tilde{\vartheta}) = \mathrm{argmin}_{(\lambda,\vartheta)\in\mathbb{R}^2} r(\lambda,\vartheta)$, whence $\nabla r(\tilde{\lambda},\tilde{\vartheta}) = 0$.

Claim 2. *$\tilde{\lambda}, \tilde{\vartheta} > 0$ and $\langle (I - P_A)u^\ell, e_\ell\rangle = (u^\ell - \tilde{z})_\ell = u^\ell_\ell - v^{J_q}(\tilde{\lambda},\tilde{\vartheta})_\ell < 0$.*

Proof of Claim 2. It suffices to show that if $(\lambda,\vartheta) \in \mathbb{R}^2$ is such that either $\lambda \leq 0$, $\vartheta \leq 0$ or $u^\ell_\ell - v^{J_q}(\lambda,\vartheta)_\ell \geq 0$, then $\nabla r(\lambda,\vartheta) \neq 0$. For any such (λ,ϑ), it is enough to prove that there exist $\lambda', \vartheta' \in \mathbb{R}$ such that $\lambda\lambda' \geq 0$, $\vartheta\vartheta' \geq 0$ and $\big(u^\ell_i - v^{J_q}_i(\lambda,\vartheta)\big)\big((1 - t^{J_q}_i)\lambda' + t^{J_q}_i\vartheta'\big) \geq 0$ for all $i \in J_q$, with at least one of these inequalities being strict, since then

$$\nabla r(\lambda,\vartheta)^\top\begin{pmatrix}\lambda'\\ \vartheta'\end{pmatrix} = 2\lambda\lambda'\,\|\tilde{v}^{J^+_q}\|^2 + 2\sum_{i \in J_q}\big(u^\ell_i - v^{J_q}_i(\lambda,\vartheta)\big)\big((1 - t^{J_q}_i)\lambda' + t^{J_q}_i\vartheta'\big) + 2\vartheta\vartheta'\,\|\tilde{v}^{J^-_q}\|^2 > 0$$

by (3.6.5). To this end, define the convex function $g \colon x \mapsto (x - x_\ell)^+$ on $[x_{a_q}, x_{a_{q-1}}]$, and let h be the unique affine function with $h(x_{a_{q-1}}) = g(x_{a_{q-1}}) - \lambda$ and $h(x_{a_q}) = g(x_{a_q}) - \vartheta$, so that $g(x_i) = u^\ell_i$ and $h(x_i) = v^{J_q}_i(\lambda,\vartheta)$ for $a_q \leq i \leq a_{q-1}$. Since (λ,ϑ) satisfies at least one of the three conditions above, the possibilities for $I := \{x \in (x_{a_q}, x_{a_{q-1}}) : h(x) > g(x)\}$ are as follows. In each case, we verify that there is an affine function $\tilde{h}$ such that $\big(g(x) - h(x)\big)\big(h(x) - \tilde{h}(x)\big) \geq 0$ for all $x \in [x_{a_q}, x_{a_{q-1}}]$, with strict inequality for some $x \in \{x_{a_q}, x_{a_q+1}, \dots, x_{a_{q-1}}\}$:

- $I = \emptyset$: then $g(x) \geq h(x)$ for all $x \in [x_{a_q}, x_{a_{q-1}}]$, and strict inequality holds for some $x \in \{x_{a_q}, x_{a_q+1}, \dots, x_{a_{q-1}}\}$, so we can take $\tilde{h}$ to be any affine function such that $\tilde{h} < h$ on $[x_{a_q}, x_{a_{q-1}}]$.

- $I = (x_{a_q}, x_{a_{q-1}})$: by the continuity of g, h, we have $g(x) \leq h(x)$ for all $x \in [x_{a_q}, x_{a_{q-1}}]$, with strict inequality for some $x \in \{x_{a_q}, x_{a_q+1}, \ldots, x_{a_{q-1}}\}$, and we can take $\tilde{h}$ to be any affine function such that $\tilde{h} > h$ on $[x_{a_q}, x_{a_{q-1}}]$.

- $I = (x_{a_q}, \tilde{x})$ for some $\tilde{x} \in (x_{a_q}, x_{a_{q-1}})$: by continuity, $g(\tilde{x}) = h(\tilde{x})$, and we must have $g(x_{a_{q-1}}) > h(x_{a_{q-1}})$ since $I \neq (x_{a_q}, x_{a_{q-1}})$. Thus, we can take $\tilde{h}$ to be any affine function satisfying $\tilde{h}(\tilde{x}) = h(\tilde{x})$ and $\tilde{h}(x_{a_q}) > h(x_{a_q})$, so that $g \leq h \leq \tilde{h}$ on $[x_{a_q}, \tilde{x}]$, $g \geq h \geq \tilde{h}$ on $[\tilde{x}, x_{a_{q-1}}]$ and $g(x_{a_{q-1}}) > h(x_{a_{q-1}}) > \tilde{h}(x_{a_{q-1}})$.

- $I = (\tilde{x}, x_{a_{q-1}})$ for some $\tilde{x} \in (x_{a_q}, x_{a_{q-1}})$: similarly, we can take $\tilde{h}$ to be any affine function satisfying $\tilde{h}(\tilde{x}) = h(\tilde{x})$ and $\tilde{h}(x_{a_{q-1}}) > h(x_{a_{q-1}})$.

Now let $\lambda' := (h - \tilde{h})(x_{a_q})$ and $\vartheta' := (h - \tilde{h})(x_{a_{q-1}})$. Then for each $i \in J_q$, we have $(h - \tilde{h})(x_i) = (1 - t_i^{J_q})\lambda' + t_i^{J_q}\vartheta'$ since $h - \tilde{h}$ is an affine function, and recall that $(g - h)(x_i) = u_i^\ell - v_i^{J_q}(\lambda, \vartheta)$. Thus, λ', ϑ' have the required properties. □

In conclusion, by the observation after (3.6.4) and Claim 2, we have

$$\operatorname{sgn}\bigl(\langle (I - P_A)u^\ell, e_{a_s}\rangle\bigr) = \operatorname{sgn}\bigl((u^\ell - \tilde{z}(\tilde{\lambda}, \tilde{\vartheta}))_{a_s}\bigr) = \begin{cases} \operatorname{sgn}\bigl(\tilde{\lambda}\tilde{v}_{a_s}^{J_q^+}\bigr) = \operatorname{sgn}\bigl(\tilde{v}_{a_s}^{J_q^+}\bigr) & \text{if } q \leq s \leq m \\ \operatorname{sgn}\bigl(\tilde{\vartheta}\tilde{v}_{a_s}^{J_q^-}\bigr) = \operatorname{sgn}\bigl(\tilde{v}_{a_s}^{J_q^-}\bigr) & \text{if } 0 \leq s \leq q-1, \end{cases}$$

which together with Claim 1 implies (3.6.2), as desired. □

Proof of Proposition 3.6.2. For fixed $A \subseteq [j-1]$ and $\ell \in [j-1]$, let $\hat{\lambda}_\ell^A(u) = \lambda_\ell(P_A u)$ and $\hat{\zeta}_\ell^A(u) = \langle u^\ell, (I - P_A)u\rangle$ be as in (3.5.12), where u is some positive multiple of e_j. Enumerate the elements of A as $j = a_0 > a_1 > \cdots > a_m > a_{m+1} = 0$ and let $q' := \min(\{2 \leq \tilde{q} \leq m : a_{\tilde{q}-1} = a_{\tilde{q}} + 1\} \cup \{m+1\})$. Now $P_A u \in \mathcal{L}_A$, and if $j - 1 \notin A$, then for all $s \in \{0, \ldots, m\}$, it follows by taking $\ell = j-1$ and $q = 1$ in (3.6.2) that

$$\langle P_A u, e_{a_s}\rangle \begin{cases} > 0 & \text{if } s < q' \text{ and } s \text{ is odd} \\ < 0 & \text{if } s < q' \text{ and } s \text{ is even} \\ = 0 & \text{if } s \geq q'. \end{cases}$$

For $\ell \in [j-1]$, we deduce from this and (3.5.9) that

$$\hat{\lambda}_\ell^A(u) = \lambda_\ell(P_A u) \begin{cases} > 0 & \text{if } \ell = a_s \text{ for some odd } 1 \leq s \leq q' \\ < 0 & \text{if } \ell = a_s \text{ for some even } 1 \leq s \leq q' \\ = 0 & \text{otherwise.} \end{cases} \tag{3.6.6}$$

Moreover, if $j - 1 \notin A$, then for $\ell \in [j-1]$, it follows by taking $s = 0$ in (3.6.2) that

$$\hat{\zeta}_\ell^A(u) = \langle (I - P_A)u^\ell, u\rangle \begin{cases} > 0 & \text{if } a_q < \ell < a_{q-1} \text{ for some odd } q \in [q'] \\ < 0 & \text{if } a_q < \ell < a_{q-1} \text{ for some even } q \in [q'] \\ = 0 & \text{if } \ell \leq a_{q'} = \ell_r \text{ or } \ell \in A. \end{cases} \tag{3.6.7}$$

We are now in a position to show that under modification (IV'), Algorithm 2 cannot remain indefinitely at any of the thresholds t_r. To this end, it suffices to verify that if $r \in \mathbb{N}$ is such that $t_r = t_{r+1} = t_{r+2}$, then $\ell_{\max} := \max(A_r^- \cup A_r^+) > \max(A_{r+1}^- \cup A_{r+1}^+)$. First, we prove that $\ell_{\max} \notin A_{r+1}^- \cup A_{r+1}^+$. Enumerating the elements of $A \equiv A_r$ as $a_1 > \cdots > a_m$ and defining a_0, q' as above, we consider separately the cases $\ell_{\max} \in A_r^-$ and $\ell_{\max} \in A_r^+$.

- If $\ell_{\max} \in A_r^-$, then $\beta_{\ell_{\max}}(t_{r+1}) = 0$ and $\hat{\lambda}_{\ell_{\max}}^{A_r}(u) > 0$. This means that $\ell_{\max} = a_s$ for some odd $s \in [q']$. Indeed, when $j-1 \notin A_r$, this follows from (3.6.6), and otherwise if $j-1 \in A_r$, then $A_r^- = \{j-1\}$ and $\ell_{\max} = j-1 = a_1$. Now $A_{r+1} = A_r \setminus \{\ell_{\max}\} \subseteq [j-2]$ under (IV'), so $\ell_{\max} \notin A_{r+1}^- \subseteq A_{r+1}$, and enumerating the elements of A_{r+1} as $a_1 > \cdots > a_{s-1} > a'_s > a'_{s+1} > \cdots > a'_{m-1}$, we have $a'_s < \ell_{\max} < a_{s-1}$. Since s $(\leq q')$ is odd, we deduce from (3.6.7) that $\hat{\zeta}_{\ell_{\max}}^{A_{r+1}}(u) > 0$, and hence that $\ell_{\max} \notin A_{r+1}^+$.
- Otherwise, if $\ell_{\max} \in A_r^+$, then $\gamma_{\ell_{\max}}(t_{r+1}) = 0$ and $\hat{\zeta}_{\ell_{\max}}^{A_r}(u) < 0$. In this case, we necessarily have $j-1 \notin A_r$, since otherwise $A_r^+ = \emptyset$, so it follows from (3.6.7) that $a_s < \ell_{\max} < a_{s-1}$ for some even $s \in [q'-1]$. Now $A_{r+1} = A_r \cup \{\ell_{\max}\} \subseteq [j-2]$ under (IV'), so $\ell_{\max} \notin A_{r+1}^+ \subseteq A_{r+1}^c$, and A_{r+1} can be enumerated as $a_1 > \cdots > a_{s-1} > a'_s > a'_{s+1} > \cdots > a'_{m+1}$, where $a'_s = \ell_{\max}$. Since s is even, we deduce from (3.6.6) that $\hat{\lambda}_{\ell_{\max}}^{A_{r+1}}(u) \leq 0$, and hence that $\ell_{\max} \notin A_{r+1}^-$.

It remains to show that $A_{r+1}^- \cup A_{r+1}^+$ does not contain any $\ell \in \{\ell_{\max}+1, \dots, j-1\}$. If $\ell_{\max} = j-1$, then there is nothing to prove, so we assume that $\ell_{\max} < j-1$, in which case $j-1 \notin A_r$ by the arguments above. Writing a'_q for the q^{th} largest element of A_{r+1}, we see that in both cases above, $a'_1 = a_1 > \cdots > a'_{s-1} = a_{s-1}$ are precisely the indices in A_{r+1} that are strictly greater than $\ell_{\max}$, where $s \leq q'$. Now fix $j-1 \geq \ell > \ell_{\max}$ and note that since $t_{r+1} = t_{r+2}$ by assumption, we have the following:

- Suppose that $\ell \in A_{r+1}$ and $\beta_\ell(t_{r+2}) = 0$, in which case $\beta_\ell(t_{r+1}) = 0$, $\ell \in A_r$ and $\ell \notin A_r^-$ by the definition of $\ell_{\max}$. Thus, $\hat{\lambda}_\ell^{A_r}(u) \leq 0$, so by applying (3.6.6) to A_r, we deduce that $\ell \neq a_q$ for any odd $q \in [q']$. Since $a_q = a'_q$ for $q \leq s-1$ and $\ell > a'_q$ for $q \geq s$, this means that $\ell \neq a'_q$ for any odd q. Applying (3.6.6) once again to A_{r+1}, we conclude that $\hat{\lambda}_\ell^{A_{r+1}}(u) \leq 0$, whence $\ell \notin A_{r+1}^-$.
- Suppose that $\ell \notin A_{r+1}$ and $\gamma_\ell(t_{r+2}) = 0$, in which case $\gamma_\ell(t_{r+1}) = 0$, $\ell \notin A_r$ and $\ell \notin A_r^+$ by the definition of $\ell_{\max}$. Thus, $\hat{\zeta}_\ell^{A_r}(u) \geq 0$, so in view of (3.6.7), we cannot have $a_q < \ell < a_{q-1}$ for any even $q \in [q'-1]$. As above, it follows that we cannot have $a'_q < \ell < a'_{q-1}$ for any even q. Applying (3.6.7) once again to A_{r+1}, we conclude that $\hat{\zeta}_\ell^{A_{r+1}}(u) \geq 0$, whence $\ell \notin A_{r+1}^+$.

This completes the justification of (IV'). Finally, we obtain both assertions of Proposition 3.6.2 as straightforward consequences of (3.6.6) and (3.6.7).

(a) By taking $q = 1$ in the first line of (3.6.7), we see that $\hat{\lambda}_\ell^{A_r}(u) > 0$ for all $\max A_r = a_1 < \ell \leq j-1$. Thus, in Algorithm 2 with modification (IV'), $A_{r+1} \subseteq A_r \cup A_r^+ \subseteq \{1, \dots, \max A_r\}$.

(b) Since $\ell_r = a_{q'}$ here, this follows immediately from the final lines of (3.6.6) and (3.6.7). □

3.6.2 Auxiliary results for Section 3.5.3

Auxiliary results for Theorem 3.3.1

The proof of Theorem 3.3.1 relies on the following bound on the localised Gaussian widths of the cone $\Gamma[\mathcal{D}] = \big\{\big(f(x_1), \dots, f(x_n)\big) : f \in \mathcal{F}\big\} \subseteq \mathbb{R}^n$, where $\mathcal{D}$ is a set of design points $x_1 < \cdots < x_n$ in $[0,1]$ and $\mathcal{F}$ is the class of all S-shaped functions on $[0,1]$. For $\theta \equiv (\theta_1, \dots, \theta_n) \in \mathbb{R}^n$ and $r > 0$, recall from Section 3.5.3 that we defined $V(\theta) = \theta_n - \theta_1$ and $\Gamma(\theta, r) \equiv \Gamma(\theta, r)[\mathcal{D}] = \{v \in \Gamma[\mathcal{D}] : \|v - \theta\| \leq r\}$.

Lemma 3.6.4. *For a set $\mathcal{D} \subseteq [0,1]$ of design points $x_1 < \cdots < x_n$ with $n \geq 2$, define $\tilde{R}(\mathcal{D})$ as in (3.5.14). Fix $\theta \in \Gamma[\mathcal{D}]$ and $r > 0$. If $Z \sim N_n(0, I_n)$, then for all $\tilde{C} \geq 1$, we have*

$$\begin{aligned}
\mathbb{E}\bigg(\sup_{v \in \Gamma(\theta, r)} |Z^\top(v - \theta)|\bigg) &\lesssim \frac{r^2}{\tilde{C}} + r\sqrt{\log n} + \big(V(\theta) + \tilde{C}\big)^{1/4} \tilde{R}(\mathcal{D})^{1/8}\, r^{3/4} \\
&\lesssim \frac{r^2}{\tilde{C}} + r\sqrt{\log n} + \big(V(\theta) + \tilde{C}\big)^{1/4} \bigg(\frac{x_n - x_1}{\min_{2 \leq i \leq n}(x_i - x_{i-1})}\bigg)^{1/8} r^{3/4}.
\end{aligned} \tag{3.6.8}$$

We will derive this result from the bounds in Lemma 3.6.5 and 3.6.6 on the covering numbers of

$$\Gamma_{A,B}[\mathcal{D}] := \{(v_1,\dots,v_n) \in \Gamma[\mathcal{D}] : A \le v_i \le B \text{ for all } i\}$$
$$K_{A,B}[\mathcal{D}] := \bigl\{\bigl(f(x_1),\dots,f(x_n)\bigr),\ f \text{ is convex },\ A \le f \le B\bigr\},$$

where $-\infty < A < B < \infty$. For $\varepsilon > 0$ and $U \subseteq \mathbb{R}^n$, recall that $\mathcal{N} \subseteq \mathbb{R}^n$ is said to be an ε-*cover* of U (with respect to the Euclidean norm $\|\cdot\|$) if $U \subseteq \bigcup_{u\in\mathcal{N}} \bar{B}(u,\varepsilon)$, where $\bar{B}(u,\varepsilon) := \{v \in \mathbb{R}^n : \|v-u\| \le \varepsilon\}$. We denote by $N(\varepsilon, U) := \inf\{|\mathcal{N}| : \mathcal{N} \text{ is an } \varepsilon\text{-cover of } U\} \in \mathbb{N}\cup\{\infty\}$ the ε-*covering number* of U.

Lemma 3.6.5. *In the setting of Lemma 3.6.4, the following holds for all $-\infty < A < B < \infty$ and $\varepsilon > 0$:*

$$\log N(\varepsilon, \Gamma_{A,B}[\mathcal{D}]) \lesssim \log n + (B-A)^{1/2}\,\frac{\tilde{R}(\mathcal{D})^{1/4}}{\varepsilon^{1/2}}. \tag{3.6.9}$$

Lemma 3.6.6. *For any finite set $\mathcal{D} \subseteq [0,1]$ and every $\varepsilon > 0$, we have*

$$\log N(\varepsilon, K_{0,1}[\mathcal{D}]) \lesssim \frac{\tilde{R}(\mathcal{D})^{1/4}}{\varepsilon^{1/2}}. \tag{3.6.10}$$

We first give the proof of (3.6.10), which gives rise to the definition of $\tilde{R}(\mathcal{D})$ in (3.5.14), and then deduce Lemmas 3.6.5 and 3.6.4 in that order.

Proof of Lemma 3.6.6. We proceed by induction on $n = |\mathcal{D}|$: for $n = 1$, the bound clearly holds since $\tilde{R}(\mathcal{D}) = 1$ by definition, so suppose now that $\mathcal{D} = \{x_1 < \cdots < x_n\}$ for some $n \ge 2$. First, by taking $c_1 = n\min_{2\le i\le n}(x_i - x_{i-1})$ in the second bound in Guntuboyina and Sen (2013, Lemma A.4) and then arguing as in the proof of Chatterjee (2016, Lemma 3.3) Chatterjee (2016, Lemma 3.3), we see that

$$\log N(\varepsilon, K_{0,1}[\mathcal{D}]) \lesssim \frac{1}{\varepsilon^{1/2}}\biggl(\frac{(x_n - x_1)}{\min_{2\le i\le n}(x_i - x_{i-1})}\biggr)^{1/4}. \tag{3.6.11}$$

In addition, for a fixed partition of $\mathcal{D}$ into $k \ge 2$ non-empty sets $\mathcal{D}_1,\dots,\mathcal{D}_k$, we define $\tilde{a}_\ell := \tilde{R}(\mathcal{D}_\ell)^{1/10}/\bigl(\sum_{\ell'=1}^k \tilde{R}(\mathcal{D}_{\ell'})^{1/5}\bigr)^{1/2}$ for $\ell \in [k]$. Given $\varepsilon > 0$, let $\varepsilon_\ell := \varepsilon\tilde{a}_\ell$ for each ℓ, so that $\varepsilon^2 = \sum_{\ell=1}^k \varepsilon_\ell^2$. Then since $|\mathcal{D}_1|,\dots,|\mathcal{D}_k| < |\mathcal{D}|$, it follows by induction that

$$\log N(\varepsilon, K_{0,1}[\mathcal{D}]) \le \sum_{\ell=1}^k \log N(\varepsilon_\ell, K_{0,1}[\mathcal{D}_\ell]) \lesssim \sum_{\ell=1}^k \frac{\tilde{R}(\mathcal{D}_\ell)^{1/4}}{\varepsilon_\ell^{1/2}} = \frac{\bigl(\sum_{\ell=1}^k \tilde{R}(\mathcal{D}_\ell)^{1/5}\bigr)^{5/4}}{\varepsilon^{1/2}}, \tag{3.6.12}$$

where by Lemma 3.6.7 below (with $b_\ell = \tilde{R}(\mathcal{D}_\ell)^{1/2}$ for all ℓ), our choice of $\varepsilon_1,\dots,\varepsilon_k$ minimises the penultimate expression above subject to the constraint $\varepsilon^2 = \sum_{\ell=1}^k \varepsilon_\ell^2$. Minimising the right hand side of (3.6.12) over all partitions of $\mathcal{D}$ into $k \ge 2$ non-empty subsets, we can combine (3.6.11) and (3.6.12) to complete the inductive step for (3.6.10), in view of the definition of $\tilde{R}(\mathcal{D})$ in (3.5.14). □

Lemma 3.6.7. *For fixed $b_1,\dots,b_k > 0$, the unique solution to the optimisation problem*

$$\min \sum_{\ell=1}^k \Bigl(\frac{b_\ell}{a_\ell}\Bigr)^{1/2} \quad \textit{subject to} \quad \sum_{\ell=1}^k a_\ell^2 = 1,\ a_\ell > 0 \textit{ for } \ell \in [k]$$

is given by $\sum_{\ell=1}^k (b_\ell/a_\ell^*)^{1/2} = \bigl(\sum_{\ell=1}^k b_\ell^{2/5}\bigr)^{5/4}$, where $a_\ell^* := b_\ell^{1/5}/\bigl(\sum_{\ell=1}^k b_\ell^{2/5}\bigr)^{1/2}$ for each ℓ.

Proof of Lemma 3.6.7. Let $\tau = 2/5$, $p = 2/(2-\tau)$ and $q = 2/\tau$, so that $1/p + 1/q = 1$, $\tau p = 1/2$ and $\tau q = 2$. Then by Hölder's inequality,

$$\sum_{\ell=1}^{k} b_\ell^{2/5} = \sum_{\ell=1}^{k} b_\ell^{\tau} \leq \left\{ \sum_{\ell=1}^{k} \left(\frac{b_\ell^\tau}{a_\ell^\tau} \right)^p \right\}^{1/p} \left(\sum_{\ell=1}^{k} a_\ell^{\tau q} \right)^{1/q} = \left(\sum_{\ell=1}^{k} b_\ell^{2/5} \right)^{5/4},$$

with equality if and only if $a_\ell = b_\ell^{p/(p+q)}/\lambda = b_\ell^{1/5}/\lambda$ for all ℓ, where taking $\lambda = \bigl(\sum_{\ell=1}^k b_\ell^{2/5}\bigr)^{1/2}$ ensures that $\sum_{\ell=1}^k a_\ell^2 = 1$. $\square$

Proof of Lemma 3.6.5. By a scaling argument, it suffices to show that

$$\log N(\varepsilon, \Gamma_{0,1}[\mathcal{D}]) \lesssim \log n + \frac{\tilde{R}(\mathcal{D})^{1/4}}{\varepsilon^{1/2}} \tag{3.6.13}$$

for all $\varepsilon > 0$, i.e. that (3.6.9) holds when $A = 0$ and $B = 1$. Indeed, for general $-\infty < A < B < \infty$, define the invertible affine map $L_{A,B} \colon \mathbb{R}^n \to \mathbb{R}^n$ by $L_{A,B}(v)_i := A + (B-A)v_i$ for $v \equiv (v_1, \ldots, v_n) \in \mathbb{R}^n$ and $i \in [n]$, so that $\Gamma_{A,B}[\mathcal{D}] = \{L_{A,B}(v) : v \in \Gamma_{0,1}[\mathcal{D}]\}$. If (3.6.13) holds, then for any $\varepsilon > 0$, we can find an $\varepsilon/(B-A)$-cover $\mathcal{N}$ of $\Gamma_{0,1}[\mathcal{D}]$ with $\log|\mathcal{N}| \lesssim \log n + (B-A)^{1/2}\,(\sqrt{Rn}/\varepsilon)^{1/2}$. For any $\theta \in \Gamma_{A,B}[\mathcal{D}]$, there exists $\theta^* \in \mathcal{N}$ satisfying $\|\theta - L_{A,B}(\theta^*)\| = (B-A)\|L_{A,B}^{-1}(\theta) - \theta^*\| \leq \varepsilon$, so $\mathcal{N}_{A,B} := \{L_{A,B}(v) : v \in \mathcal{N}\}$ is an ε-cover of $\Gamma_{A,B}[\mathcal{D}]$ with $\log|\mathcal{N}_{A,B}| = \log|\mathcal{N}| \lesssim \log n + (B-A)^{1/2}\,(\sqrt{Rn}/\varepsilon)^{1/2}$, as desired.

To establish (3.6.13), fix $\varepsilon > 0$ and let $\Gamma_{0,1}^m[\mathcal{D}] := \bigl\{\bigl(f(x_1), \ldots, f(x_n)\bigr) : f \in \mathcal{F}^m, 0 \leq f \leq 1\bigr\}$ for $m \in [0,1]$, so that $\Gamma_{0,1}[\mathcal{D}] = \bigcup_{j=1}^n \Gamma_{0,1}^{x_j}[\mathcal{D}]$ and $N(\varepsilon, \Gamma_{0,1}[\mathcal{D}]) \leq \sum_{i=1}^n N(\varepsilon, \Gamma_{0,1}^{x_j}[\mathcal{D}]) \leq n \max_{1 \leq j \leq n} N(\varepsilon, \Gamma_{0,1}^{x_j}[\mathcal{D}])$. Now for $j \in [n]$, let $\mathcal{D}_j^- := \{x_i : 1 \leq i \leq j\}$ and $\mathcal{D}_j^+ := \{x_i : j+1 \leq i \leq n\}$. Then $\Gamma_{0,1}[\mathcal{D}] \subseteq K_{0,1}[\mathcal{D}_j^-] \times \bigl(-K_{0,1}[\mathcal{D}_j^+]\bigr)$ and $\tilde{R}(\mathcal{D}_j^\pm) \leq \tilde{R}(\mathcal{D})$ by (3.5.14), so it follows from Lemma 3.6.6 that

$$\log N(\varepsilon, \Gamma_{0,1}^{x_j}[\mathcal{D}]) \leq \log N\bigl(\varepsilon/\sqrt{2}, K_{0,1}[\mathcal{D}_j^-]\bigr) + \log N\bigl(\varepsilon/\sqrt{2}, K_{0,1}[\mathcal{D}_j^+]\bigr) \lesssim \frac{\tilde{R}(\mathcal{D})^{1/4}}{\varepsilon^{1/2}}.$$

We conclude that

$$\log N(\varepsilon, \Gamma_{0,1}[\mathcal{D}]) \leq \log n + \max_{1 \leq j \leq n} \log N(\varepsilon_\ell, \Gamma_{0,1}^{x_j}[\mathcal{D}]) \lesssim \log n + \frac{\tilde{R}(\mathcal{D})^{1/4}}{\varepsilon^{1/2}},$$

as required. $\square$

When $\varepsilon \gg B - A$, it turns out that in the proof above, we do not have to construct separate ε-covers for each of the sets $\Gamma_{A,B}^{x_1}[\mathcal{D}], \ldots, \Gamma_{A,B}^{x_n}[\mathcal{D}]$ individually. This is because elements of $\Gamma_{A,B}^{x_j}[\mathcal{D}]$ can be approximated to accuracy ε by those in a covering set for $\Gamma_{A,B}^{x_{j'}}[\mathcal{D}]$ with j' close to j. In general, we can improve the first $\log n$ term in (3.6.9) to $\log\bigl(1 \vee \{n(B-A)^2/\varepsilon^2\} \wedge n\bigr)$, and hence obtain an overall bound in Lemma 3.6.5 that tends to 0 as $\varepsilon \to \infty$. We omit further details of these additional arguments, since this improved result leads to the same worst-case oracle inequality (3.3.1) as in Theorem 3.3.1 (possibly with a slightly smaller universal constant C).

Proof of Lemma 3.6.4. Fix $\theta \in \Gamma$ and let $Z \sim N_n(0, I_n)$. For every $k \in \mathbb{N}$, let $A_k := \theta_1 - 2^k = \min_{1 \leq i \leq n} \theta_i - 2^k$ and $B_k := \theta_n + 2^k = \max_{1 \leq i \leq n} \theta_i + 2^k$, and define $\pi_k(s) := s \vee A_k \wedge B_k$ for $s \in \mathbb{R}$. Note that if $v \in \Gamma$, then $\pi_k(v) := (\pi_k(v_1), \ldots, \pi_k(v_n)) \in \Gamma_{A_k, B_k} =: \tilde{\Gamma}_k$. Moreover, $\theta \in \tilde{\Gamma}_k$ in view of our choice of A_k, B_k, and if $v \in \Gamma(\theta, r)$ for some $r > 0$, then $\pi_k(v) \in \tilde{\Gamma}_k(\theta, r)$. Consequently, for any

$r > 0$ and $k \in \mathbb{N}$, we have

$$\begin{aligned}\mathbb{E}\biggl(\sup_{v\in\Gamma(\theta,r)} |Z^\top(v-\theta)|\biggr) &\leq \mathbb{E}\biggl(\sup_{v\in\Gamma(\theta,r)} \bigl|Z^\top\bigl(\pi_k(v)-\theta\bigr)\bigr|\biggr) + \mathbb{E}\biggl(\sup_{v\in\Gamma(\theta,r)} \bigl|Z^\top\bigl(v-\pi_k(v)\bigr)\bigr|\biggr)\\ &\leq \mathbb{E}\biggl(\sup_{u\in\tilde{\Gamma}_k(\theta,r)} |Z^\top(u-\theta)|\biggr) + \mathbb{E}\biggl(\sup_{v\in\Gamma(\theta,r)} \bigl|Z^\top\bigl(v-\pi_k(v)\bigr)\bigr|\biggr). \end{aligned} \tag{3.6.14}$$

To bound the first term in (3.6.14), observe first that by the triangle inequality, $\tilde{\Gamma}_k(\theta,r)$ has diameter $d := \sup\{\|v-v'\| : v, v' \in \tilde{\Gamma}_k(\theta,r)\} \leq 2r$. We can now apply Lemma 3.6.5 in conjunction with Dudley's metric entropy bound for Gaussian processes (e.g. Giné and Nickl, 2016, Theorem 2.3.7) to see that

$$\begin{aligned}\mathbb{E}\biggl(\sup_{u\in\tilde{\Gamma}_k(\theta,r)} |Z^\top(u-\theta)|\biggr) &\leq 4\sqrt{2}\int_0^{d/2} \sqrt{\log 2N\bigl(\varepsilon,\tilde{\Gamma}_k(\theta,r)\bigr)}\,d\varepsilon \leq 4\sqrt{2}\int_0^{r} \sqrt{\log 2N(\varepsilon,\Gamma_{A_k,B_k})}\,d\varepsilon\\ &\lesssim \int_0^r \bigl\{\sqrt{\log n} + (B_k-A_k)^{1/4}\tilde{R}(\mathcal{D})^{1/8}\,\varepsilon^{-1/4}\bigr\}\,d\varepsilon\\ &\lesssim r\sqrt{\log n} + \bigl(V(\theta)+2^k\bigr)^{1/4}\tilde{R}(\mathcal{D})^{1/8}\,r^{3/4}. \end{aligned} \tag{3.6.15}$$

As for the second term in (3.6.14), we define $I_{1,\ell}(v) := \{1 \leq i \leq n : A_{\ell+1} < v_i \leq A_\ell\}$ and $I_{2,\ell}(v) := \{1 \leq i \leq n : B_\ell \leq v_i < B_{\ell+1}\}$ for $v \equiv (v_1,\ldots,v_n) \in \mathbb{R}^n$ and $\ell \in \mathbb{N}$. Note that if $j \in I_{1,\ell}(v)$ for some $\ell \geq k$, then $\theta_j - v_j \geq \theta_1 - A_\ell = 2^\ell$ and $0 \leq \pi_k(v_j) - v_j < \theta_1 - A_{\ell+1} = 2^{\ell+1}$. Similarly, $v_j - \theta_j \geq 2^\ell$ and $0 \leq v_j - \pi_k(v_j) < 2^{\ell+1}$ for all $j \in I_{2,\ell}(v)$. Thus, if $v \in \Gamma(\theta,r)$, then $\sum_{i=1}^n(\theta_i - v_i)^2 \leq r^2$, so $|I_{1,\ell}(v)| \vee |I_{2,\ell}(v)| \leq r^2/2^{2\ell}$; in fact, since $v_1 \leq \cdots \leq v_n$, this means that $I_{1,\ell}(v) \subseteq \{1,\ldots,\lfloor r^2/2^{2\ell}\rfloor\}$ and $I_{2,\ell}(v) \subseteq \{n+1-i : 1 \leq i \leq \lfloor r^2/2^{2\ell}\rfloor\}$. Consequently, for every $v \in \Gamma(\theta,r)$, we have

$$\begin{aligned}\bigl|Z^\top\bigl(v-\pi_k(v)\bigr)\bigr| &\leq \sum_{\ell=k}^\infty \sum_{i\in I_{1,\ell}(v)\,\cup\, I_{2,\ell}(v)} |Z_i|\,|v_i - \pi_k(v_i)| \leq \sum_{\ell=k}^\infty 2^{\ell+1} \sum_{i\in I_{1,\ell}(v)\,\cup\, I_{2,\ell}(v)} |Z_i|\\ &\leq \sum_{\ell=k}^\infty 2^{\ell+1} \sum_{i=1}^{\lfloor r^2/2^{2\ell}\rfloor} (|Z_i| + |Z_{n+1-i}|),\end{aligned}$$

so

$$\mathbb{E}\biggl(\sup_{v\in\Gamma(\theta,r)} \bigl|Z^\top\bigl(v-\pi_k(v)\bigr)\bigr|\biggr) \leq \sum_{\ell=k}^\infty 2^{\ell+2} \sum_{i=1}^{\lfloor r^2/2^{2\ell}\rfloor} \mathbb{E}(|Z_i|) \lesssim \sum_{\ell=k}^\infty \frac{r^2}{2^\ell} \lesssim \frac{r^2}{2^k}. \tag{3.6.16}$$

Finally, for any $\tilde{C} \geq 1$, let $k \in \mathbb{N}$ be such that $2^{k-1} \leq \tilde{C} < 2^k$. The desired bound (3.6.8) then follows from (3.6.14), (3.6.15) and (3.6.16). □

Auxiliary results for Theorem 3.3.3

Here, we establish the key technical Lemmas 3.5.8–3.5.10 that form part of the proof of Theorem 3.3.3, as well as Lemma 3.5.11 from the proof of Proposition 3.3.4. Lemma 3.6.8 below is the starting point for the proof of Lemma 3.5.8, and applies to general configurations of design points $x_1 < \cdots < x_n$ (which need not be equispaced).

Lemma 3.6.8. *Let x_k be a kink of the convex LSE $\hat{g}_n$ based on $(x_1,Y_1),\ldots,(x_n,Y_n)$. Let $\bar{x}_L := k^{-1}\sum_{i=1}^k x_i$ and $\bar{x} := n^{-1}\sum_{i=1}^n x_i$. Then*

$$\frac{\sum_{i=1}^k (x_i - \bar{x}_L)Y_i}{\sum_{i=1}^k (x_i-\bar{x}_L)^2} \leq \frac{\sum_{i=1}^n (x_i - \bar{x})Y_i}{\sum_{i=1}^n (x_i-\bar{x})^2}.$$

In other words, the slope of the regression line fitted using $\{(x_i, Y_i) : 1 \le i \le k\}$ is at most that of the regression line fitted using $\{(x_i, Y_i) : 1 \le i \le n\}$.

Proof. Let $S_L^2 := \sum_{i=1}^k (x_i - \bar{x}_L)^2$ and $S^2 := \sum_{i=1}^n (x_i - \bar{x})^2$. Then

$$S^2 \ge \sum_{i=1}^k (x_i - \bar{x})^2 = \sum_{i=1}^k (x_i - \bar{x}_L)^2 + k(\bar{x}_L - \bar{x})^2 \ge S_L^2 > 0,$$

since $k \ge 2$. The linear functions $h_L, h_R : \mathbb{R} \to \mathbb{R}$ defined by $h_L(x) := S_L^{-2}(x - \bar{x}_L) - S^{-2}(x - \bar{x})$ and $h_R(x) := -S^{-2}(x - \bar{x})$ have slopes $S_L^{-2} - S^{-2} \ge 0$ and $-S^{-2} < 0$ respectively. Now let $h \in \mathcal{G}$ be such that $h(x_i) = h_L(x_i)$ for $i \in [k]$ and $h(x_i) = h_R(x_i)$ for $k + 1 \le i \le n$. Since $h_L(x_k) = S_L^{-2}(x_k - \bar{x}_L) - S^{-2}(x_k - \bar{x}) \ge -S^{-2}(x_k - \bar{x}) = h_R(x_k)$, this means that h is convex on both $[x_1, x_k]$ and $[x_k, x_n]$ (and locally concave at x_k, a kink of $\hat{g}_n$). Therefore, $\hat{g}_n + \eta h \in \mathcal{G}$ is convex for sufficiently small $\eta > 0$, whence $\sum_{i=1}^n h(x_i)\bigl(Y_i - \hat{g}_n(x_i)\bigr) \le 0$ by (3.5.3) or Lemma 3.6.1.

To establish that $\sum_{i=1}^n h(x_i)\, Y_i = \sum_{i=1}^k (h_L - h_R)(x_i)\, Y_i + \sum_{i=1}^n h_R(x_i)\, Y_i \le 0$, as claimed in the lemma, it therefore suffices to show that

$$\sum_{i=1}^n h(x_i)\, \hat{g}_n(x_i) = \sum_{i=1}^k (h_L - h_R)(x_i)\, \hat{g}_n(x_i) + \sum_{i=1}^n h_R(x_i)\, \hat{g}_n(x_i) \le 0,$$

i.e. that the slope of the regression line fitted using $\{(x_i, \hat{g}_n(x_i)) : 1 \le i \le k\}$ is at most that of the regression line fitted using $\{(x_i, \hat{g}_n(x_i)) : 1 \le i \le n\}$. To this end, for $j \in [n]$, let $K^{1,j} \subseteq \mathbb{R}^j$ be the closed, convex cone of convex sequences based on $x_1, \dots, x_j$, as defined at the start of Section 3.5.3, and define $\hat{v}^j := \bigl(\hat{g}_n(x_1), \dots, \hat{g}_n(x_j)\bigr) \in K^{1,j}$. Let $\pm u^{j,0}, \pm u^{j,1}, u^{j,2}, \dots, u^{j,j-1} \in K^{1,j}$ be its generators, where $u_i^{j,0} = 1$ and $u_i^{j,\ell} = (x_i - x_\ell)^+$ for all $i \in [j]$ and $\ell \in [j-1]$ as in the paragraph containing (3.2.1). Since $\hat{v}^n \in K^{1,n}$, we can write $\hat{v}^n = \sum_{\ell=0}^{n-1} \hat{\lambda}_\ell u^\ell$ for some $\hat{\lambda}_0, \dots, \hat{\lambda}_{n-1} \in \mathbb{R}$ with $\hat{\lambda}_2, \dots, \hat{\lambda}_{n-1} \ge 0$. Let $A_L := \{0, 1\} \cup \{2 \le \ell \le k-1 : \hat{\lambda}_\ell > 0\}$ and $A_R := \{k \le \ell \le n-1 : \hat{\lambda}_\ell > 0\}$, so that

$$\hat{v}^k = \sum_{\ell \in A_L} \hat{\lambda}_\ell u^{k,\ell} \quad \text{and} \quad \hat{v}^n = \sum_{\ell \in A_L} \hat{\lambda}_\ell u^{n,\ell} + \sum_{\ell \in A_R} \hat{\lambda}_\ell u^{n,\ell}.$$

For $j \in [n]$, let $\tilde{P}_j \in \mathbb{R}^{j \times j}$ represent the orthogonal projection onto $L_j := \mathrm{span}\{u^{j,0}, u^{j,1}\}$, so that if $z \in \mathbb{R}^j$, then $\tilde{P}_j z$ is the vector of fitted values from ordinary least squares regression based on $\{(x_i, z_i) : 1 \le i \le j\}$. We say that $v \in L_j$ has *slope* b if $v_i - v_{i-1} = b(x_i - x_{i-1})$ for $2 \le i \le j$, and denote by $b_{j\ell}$ the slope of $\tilde{P}_j u^{j,\ell}$ for $0 \le \ell \le j-1$. Since $k \le n$, observe that $0 \le b_{k\ell} \le b_{n\ell} \le 1$ for all $0 \le \ell \le k-1$ and $b_{k\ell} = b_{n\ell}$ for $r \in \{0, 1\}$. Writing b_k and b_n for the slopes of $\tilde{P}_k \hat{v}^k = \sum_{\ell \in A_L} \hat{\lambda}_\ell \tilde{P}_k u^{k,\ell}$ and $\tilde{P}_n \hat{v}^n = \sum_{\ell \in A_L} \hat{\lambda}_\ell \tilde{P}_n u^{n,\ell} + \sum_{\ell \in A_R} \hat{\lambda}_\ell \tilde{P}_n u^{n,\ell}$ respectively, we conclude that

$$b_k = \sum_{\ell \in A_L} \hat{\lambda}_\ell\, b_{k\ell} \le \sum_{\ell \in A_L} \hat{\lambda}_\ell\, b_{n\ell} + \sum_{\ell \in A_R} \hat{\lambda}_\ell\, b_{n\ell} = b_n.$$

This completes the proof. □

Proof of Lemma 3.5.8. If $\hat{\tau}_{0L} \neq m_0$ (i.e. $\{i : x_i \in \mathcal{I}_{01}\}$ is non-empty), then $\hat{\tau}_{0L}$ is a kink of $\hat{g}_{n,0}$ in $(m_0, (m_0 + \tilde{m}_+)/2]$. Define $N_{01} := |\{i : x_i \in \mathcal{I}_{01}\}| \vee 1$, $N_0 := |\{i : x_i \in \mathcal{I}_0\}|$, $\bar{x}_{01} := N_{01}^{-1} \sum_{i : x_i \in \mathcal{I}_{01}} x_i$ and $\bar{x}_0 := N_0^{-1} \sum_{i : x_i \in \mathcal{I}_0} x_i$, where we suppress the dependence on n for convenience. We deduce from Lemma 3.6.8 that if $N_{01} \ge 2$, then

$$\frac{\sum_{i : x_i \in \mathcal{I}_{01}} (x_i - \bar{x}_{01}) Y_i}{\sum_{i : x_i \in \mathcal{I}_{01}} (x_i - \bar{x}_{01})^2} \le \frac{\sum_{i : x_i \in \mathcal{I}_0} (x_i - \bar{x}_0) Y_i}{\sum_{i : x_i \in \mathcal{I}_0} (x_i - \bar{x}_0)^2},$$

and hence that

$$\frac{\sum_{i:x_i\in\mathcal{I}_{01}}(x_i-\bar{x}_{01})f_0(x_i)}{\sum_{i:x_i\in\mathcal{I}_{01}}(x_i-\bar{x}_{01})^2}-\frac{\sum_{i:x_i\in\mathcal{I}_{0}}(x_i-\bar{x}_{0})f_0(x_i)}{\sum_{i:x_i\in\mathcal{I}_{0}}(x_i-\bar{x}_{0})^2}$$
$$\leq\frac{\sum_{i:x_i\in\mathcal{I}_{0}}(x_i-\bar{x}_{0})\,\xi_i}{\sum_{i:x_i\in\mathcal{I}_{0}}(x_i-\bar{x}_{0})^2}-\frac{\sum_{i:x_i\in\mathcal{I}_{01}}(x_i-\bar{x}_{01})\,\xi_i}{\sum_{i:x_i\in\mathcal{I}_{01}}(x_i-\bar{x}_{01})^2}. \tag{3.6.17}$$

Let β_{L1},β_{L2} be equal to the first and second terms respectively on the right-hand side of (3.6.17) when $N_{01}\geq 2$ (and set $\beta_{L1}=\beta_{L2}=0$ otherwise). Taking into account the randomness of the intervals $\mathcal{I}_{01},\mathcal{I}_0$, we claim that $(\beta_{L1}-\beta_{L2})\sqrt{n(\hat{\tau}_{0L}-m_0)^3}=O_p(\sqrt{\log n})$. Indeed, for fixed $1\leq a<b\leq n$, define $\bar{x}_{a:b}:=(b-a+1)^{-1}\sum_{i=a}^b x_i$, $S_{ab}^2:=\sum_{i=a}^b(x_i-\bar{x}_{a:b})^2$ and $\tilde{\beta}_{ab}:=S_{ab}^{-2}\sum_{i=a}^b(x_i-\bar{x}_{a:b})\,\xi_i$. Under Assumption 2, the design points $x_i\equiv x_{ni}=i/n$ are equispaced and the errors ξ_i are sub-Gaussian with parameter 1, so $S_{ab}^2\asymp(b-a)^3/n^2$ and $\tilde{\beta}_{ab}$ has sub-Gaussian parameter $S_{ab}^{-2}\asymp n^2/(b-a)^3=n^{-1}(x_b-x_a)^{-3}$. Therefore, $\tilde{\beta}_{\max}:=\max_{1\leq a<b\leq n}|\tilde{\beta}_{ab}|\sqrt{n(x_b-x_a)^3}=O_p(\sqrt{\log n})$ (e.g. Giné and Nickl, 2016, Lemma 2.3.4), so

$$\sqrt{n(\hat{\tau}_{0L}-m_0)^3}\,|\beta_{L1}|\leq 2^{3/2}\,\tilde{\beta}_{\max}=O_p(\sqrt{\log n})$$
$$\sqrt{n(\hat{\tau}_{0L}-m_0)^3}\,|\beta_{L2}|\leq\sqrt{n(\tilde{m}_+-m_0)^3}\,|\beta_{L2}|\leq 2^{3/2}\,\tilde{\beta}_{\max}=O_p(\sqrt{\log n}), \tag{3.6.18}$$

which justifies the claim above. Now let b_{L1},b_{L2} be equal to the first and second terms respectively on the left-hand side of (3.6.17) when $N_{01}\geq 2$ (and set $b_{L1}=b_{L2}=0$ otherwise). For $\gamma>1$ and $x_a\in(m_0,1]$, let $s_\gamma(x_a):=n^{-1}\sum_{i:x_i\in(m_0,x_a]}(x_i-m_0)^\gamma$, and observe that if $x_{j-1}\leq m_0<x_j<x_a$, then

$$\frac{(x_a-m_0)^{\gamma+1}}{\gamma+1}\leq\int_{x_{j-1}}^{x_a}(x-m_0)^\gamma\,dx\leq s_\gamma(x_a)\leq\int_{x_j}^{x_{a+1}}(x_a\wedge x-m_0)^\gamma\,dx$$
$$\leq\frac{(x_a-m_0)^{\gamma+1}}{\gamma+1}\biggl(1+\frac{\gamma+1}{n(x_a-m_0)}\biggr). \tag{3.6.19}$$

We claim that if $\hat{\tau}_{0L}-m_0\geq 2n^{-1/(2\alpha+1)}$, then

$$\begin{aligned}b_{L1}&=f_0'(m_0)-B\bigl(1+o_p(1)\bigr)\,\frac{s_{\alpha+1}(\hat{\tau}_{0L})-2^{-1}s_\alpha(\hat{\tau}_{0L})(\hat{\tau}_{0L}-m_0)}{s_2(\hat{\tau}_{0L})-2^{-1}s_1(\hat{\tau}_{0L})(\hat{\tau}_{0L}-m_0)}\\&\geq f_0'(m_0)-\frac{6\alpha B}{(\alpha+1)(\alpha+2)}\bigl(1+o_p(1)\bigr)(\hat{\tau}_{0L}-m_0)^{\alpha-1}\end{aligned} \tag{3.6.20}$$

and

$$\begin{aligned}b_{L2}&=f_0'(m_0)-B\bigl(1+o_p(1)\bigr)\,\frac{s_{\alpha+1}(\tilde{m}_+)-2^{-1}s_\alpha(\tilde{m}_+)(\tilde{m}_+-m_0)}{s_2(\tilde{m}_+)-2^{-1}s_1(\tilde{m}_+)(\tilde{m}_+-m_0)}\\&\leq f_0'(m_0)-\frac{6\alpha B}{(\alpha+1)(\alpha+2)}\bigl(1+o_p(1)\bigr)(\tilde{m}_+-m_0)^{\alpha-1}\\&\leq f_0'(m_0)-2^{\alpha-1}\frac{6\alpha B}{(\alpha+1)(\alpha+2)}\bigl(1+o_p(1)\bigr)(\hat{\tau}_{0L}-m_0)^{\alpha-1}.\end{aligned} \tag{3.6.21}$$

To see this, recall that under (3.3.5) in Assumption 2, we can write $f_0(x)=f_0(m_0)+f_0'(m_0)(x-m_0)-B\bigl(1+\eta(x-m_0)\bigr)\operatorname{sgn}(x-m_0)|x-m_0|^\alpha$ for $x\in[0,1]$ when $\alpha>1$, where $\eta(x-m_0)\to 0$ as

$x \to m_0$. Writing $x_i - \bar{x}_{01} = (x_i - m_0) - 2^{-1}(\hat{\tau}_{0L} - m_0)$, we see that

$$\begin{aligned}\textstyle\sum_{i:x_i\in\mathcal{I}_{01}}(x_i - \bar{x}_{01})\bigl(f_0(m_0) + f_0'(m_0)(x_i - m_0)\bigr) &= f_0'(m_0)\textstyle\sum_{i:x_i\in\mathcal{I}_{01}}(x_i - \bar{x}_{01})(x_i - m_0)\\ &= f_0'(m_0)\bigl(s_2(\hat{\tau}_{0L}) - 2^{-1}s_1(\hat{\tau}_{0L})(\hat{\tau}_{0L} - m_0)\bigr) \qquad (3.6.22)\\ &= f_0'(m_0)\textstyle\sum_{i:x_i\in\mathcal{I}_{01}}(x_i - \bar{x}_{01})^2\end{aligned}$$

and $$\textstyle\sum_{i:x_i\in\mathcal{I}_{01}}(x_i - \bar{x}_{01})(x_i - m_0)^\alpha = s_{\alpha+1}(\hat{\tau}_{0L}) - 2^{-1}s_\alpha(\hat{\tau}_{0L}). \qquad (3.6.23)$$

Moreover, since $\omega(\delta) := \sup\{|\eta(x-m_0)| : x \in [0,1],\ |x-m_0| \le \delta\} \to 0$ as $\delta \to 0$ and $\tilde{m}_+ - m_0 = o_p(1)$ by Proposition 3.1.2(a), we have

$$\begin{aligned}\bigl|\textstyle\sum_{i:x_i\in\mathcal{I}_{01}}(x_i - \bar{x}_{01})\,\eta(x_i - m_0)(x_i - m_0)^\alpha\bigr| &\le \omega(|\tilde{m}_+ - m_0|)\textstyle\sum_{i:x_i\in\mathcal{I}_{01}}|x_i - \bar{x}_{01}|(x_i - m_0)^\alpha\\ &= o_p(1)\bigl(s_{\alpha+1}(\hat{\tau}_{0L}) + 2^{-1}s_\alpha(\hat{\tau}_{0L})(\hat{\tau}_{0L} - m_0)\bigr). \qquad (3.6.24)\end{aligned}$$

Combining (3.6.22), (3.6.23) and (3.6.24), we obtain the first equality in (3.6.20). On the event $\{\hat{\tau}_{0L} - m_0 \ge 2n^{-1/(2\alpha+1)}\}$, we find using (3.6.19) that

$$\begin{aligned}\frac{s_{\alpha+1}(\hat{\tau}_{0L}) - 2^{-1}s_\alpha(\hat{\tau}_{0L})(\hat{\tau}_{0L} - m_0)}{s_2(\hat{\tau}_{0L}) - 2^{-1}s_1(\hat{\tau}_{0L})(\hat{\tau}_{0L} - m_0)} &\le \frac{\frac{\alpha}{2(\alpha+1)(\alpha+2)} + \frac{1}{n(\hat{\tau}_{0L}-m_0)}}{\frac{1}{12} - \frac{1}{2n(\hat{\tau}_{0L}-m_0)}}(\hat{\tau}_{0L} - m_0)^{\alpha-1}\\ &\le \bigl(1 + o(1)\bigr)\frac{6\alpha}{(\alpha+1)(\alpha+2)}(\hat{\tau}_{0L} - m_0)^{\alpha-1},\end{aligned}$$

which justifies the lower bound on b_{L1} in (3.6.20). We can derive (3.6.21) similarly by first establishing analogues of (3.6.22), (3.6.23) and (3.6.24), and then applying (3.6.19) to see that

$$\begin{aligned}\frac{s_{\alpha+1}(\tilde{m}_+) - 2^{-1}s_\alpha(\tilde{m}_+)(\tilde{m}_+ - m_0)}{s_2(\tilde{m}_+) - 2^{-1}s_1(\tilde{m}_+)(\tilde{m}_+ - m_0)} &\ge \frac{\frac{\alpha}{2(\alpha+1)(\alpha+2)} - \frac{1}{2n(\tilde{m}_+-m_0)}}{\frac{1}{12} + \frac{1}{n(\tilde{m}_+-m_0)}}(\tilde{m}_+ - m_0)^{\alpha-1}\\ &\ge \bigl(1 + o(1)\bigr)\frac{6\alpha}{(\alpha+1)(\alpha+2)}(\tilde{m}_+ - m_0)^{\alpha-1}\end{aligned}$$

on the event $E_n^+ \supseteq \{\hat{\tau}_{0L} - m_0 \ge 2n^{-1/(2\alpha+1)}\}$. Since $\tilde{m}_+ - m_0 \ge 2(\hat{\tau}_{0L} - m_0)$ and $\alpha > 1$, this yields the upper bound on b_{L2} in (3.6.21).

Thus, on the event $\{\hat{\tau}_{0L} - m_0 \ge 2n^{-1/(2\alpha+1)}\}$, we can apply (3.6.20), (3.6.21), (3.6.17) and (3.6.18) in that order to deduce that

$$\begin{aligned}(2^{\alpha-1} - 1)\frac{6\alpha B}{(\alpha+1)(\alpha+2)}\bigl(1 + o_p(1)\bigr)\sqrt{n}(\hat{\tau}_{0L} - m_0)^{\alpha+\frac{1}{2}} &\le (b_{L1} - b_{L2})\sqrt{n(\hat{\tau}_{0L} - m_0)^3}\\ &\le (\beta_{L1} - \beta_{L2})\sqrt{n(\hat{\tau}_{0L} - m_0)^3}\\ &= O_p(\sqrt{\log n}).\end{aligned}$$

We conclude that $\hat{\tau}_{0L} - m_0 = O_p\bigl((n/\log n)^{-1/(2\alpha+1)}\bigr)$, as required. □

Proof of Lemma 3.5.9. Since $C_n \to \infty$, we have

$$t_n = \sqrt{C_n}\,(n/\log n)^{-1/(2\alpha+1)} < 4^{-1}C_n(n/\log n)^{-1/(2\alpha+1)} = u_n/2$$

for all sufficiently large n. For each n, let $a_n := \lceil n(m_0 + u_n/2)\rceil$ and $b_n := \lfloor n(m_0 + u_n)\rfloor$, so that $x_{a_n} < m_0 + u_n/2 \le x_{a_n+1}$ and $x_{b_n-1} \le m_0 + u_n < x_{b_n}$. Then for all sufficiently large n, we have $\inf_{(a,b)\in\mathcal{T}_n}\inf_{c_0,c_1}\|\theta^{a,b} - c_0\mathbf{1}^{a,b} - c_1x^{a,b}\|^2 \ge \inf_{c_0,c_1}\|\theta^{a_n,b_n} - c_0\mathbf{1}^{a_n,b_n} - c_1x^{a_n,b_n}\|^2 =: R_n$.

For $x \in [m_0, 1]$, recall from (3.3.5) in Assumption 2 that

$$f_0(x) = \begin{cases} f_0(m_0) + f_0'(m_0)(x - m_0) - B\bigl(1 + \eta(x - m_0)\bigr)(x - m_0)^\alpha & \text{when } \alpha > 1 \\ f_0(m_0) + B\bigl(1 + \eta(x - m_0)\bigr)(x - m_0)^\alpha & \text{when } \alpha \in (0, 1), \end{cases}$$

where $\eta(x - m_0) \to 0$ as $x \to m_0$. For each n, let $\widetilde{\theta}_i^{a_n, b_n} := B\bigl(1 + \eta(x_i - m_0)\bigr)(x_i - m_0)^\alpha$ for $m_0 \le a_n \le i \le b_n$ and $\widetilde{\theta}^{a_n,b_n} := \bigl(\widetilde{\theta}_{a_n}^{a_n,b_n}, \dots, \widetilde{\theta}_{b_n}^{a_n,b_n}\bigr)$, so that $\widetilde{\theta}^{a_n,b_n} + \theta^{a_n,b_n} \in \operatorname{span}\{\mathbf{1}^{a_n,b_n}, x^{a_n,b_n}\} =: A^{a_n,b_n}$ when $\alpha > 1$ and $\widetilde{\theta}^{a_n,b_n} - \theta^{a_n,b_n} \in A^{a_n,b_n}$ when $\alpha \in (0,1)$. In addition, let $\bar{x}_{a_n,b_n} := (b_n - a_n + 1)^{-1} \sum_{i=a_n}^{b_n} x_i$, so that $\widetilde{x}^{a_n,b_n} := x^{a_n,b_n} - \bar{x}_{a_n,b_n} \mathbf{1}^{a_n,b_n}$ satisfies $\langle \mathbf{1}^{a_n,b_n}, \widetilde{x}^{a_n,b_n} \rangle = 0$ and $A^{a_n,b_n} = \operatorname{span}\{\mathbf{1}^{a_n,b_n}, \widetilde{x}^{a_n,b_n}\}$. Then

$$R_n = \inf_{v \in A^{a_n,b_n}} \|\theta^{a_n,b_n} - v\|^2 = \inf_{v \in A^{a_n,b_n}} \|\widetilde{\theta}^{a_n,b_n} - v\|^2 = \|\widetilde{\theta}^{a_n,b_n}\|^2 - c_{n0}^2 \,\|\mathbf{1}^{a_n,b_n}\|^2 - c_{n1}^2 \,\|\widetilde{x}^{a_n,b_n}\|^2, \tag{3.6.25}$$

where $c_{n0} := \langle \widetilde{\theta}^{a_n,b_n}, \mathbf{1}^{a_n,b_n} \rangle / \|\mathbf{1}^{a_n,b_n}\|^2$ and $c_{n1} := \langle \widetilde{\theta}^{a_n,b_n}, \widetilde{x}^{a_n,b_n} \rangle / \|\widetilde{x}^{a_n,b_n}\|^2$. We will consider in turn the three terms on the right-hand side of (3.6.25). For each n, let $M_n := nu_n$ and $z_{n,i} := (x_i - m_0)/u_n$ for $a_n \le i \le b_n$, where $x_i \equiv x_{ni} = i/n$ by Assumption 2. Then $z_{n,i+1} - z_{n,i} = 1/M_n$ for all $a_n \le i < b_n$, and $z_{n,a_n} = 1/2 + o(1/M_n)$ and $z_{n,b_n} = 1 + o(1/M_n)$ by the definitions of a_n, b_n. Moreover, let $\tilde{\eta}_n(z) := \bigl(1 + \eta(u_n z)\bigr)^2 - 1$ for $z \in [1/2, 1]$ and note that $\sup_{z \in [1/2,1]} |\tilde{\eta}_n(z)| = o(1)$ as $n \to \infty$. The first term in (3.6.25) can now be written as

$$\begin{aligned} \|\widetilde{\theta}^{a_n,b_n}\|^2 &= \sum_{i=a_n}^{b_n} B^2 \bigl(1 + \eta(x_i - m_0)\bigr)^2 (x_i - m_0)^{2\alpha} \\ &= nu_n^{2\alpha+1} \sum_{i=a_n}^{b_n} \frac{B^2}{nu_n} \bigl(1 + \eta(x_i - m_0)\bigr)^2 \left(\frac{x_i - m_0}{u_n}\right)^{2\alpha} \\ &= B^2 nu_n^{2\alpha+1} \sum_{i=a_n}^{b_n} M_n^{-1} \bigl(1 + \tilde{\eta}_n(z_{n,i})\bigr)\, z_{n,i}^{2\alpha}. \end{aligned} \tag{3.6.26}$$

Defining $F(z) := z^\alpha$ for $z \in [1/2, 1]$ and noting that $M_n = nu_n = 2^{-1} C_n (n^{2\alpha} \log n)^{1/(2\alpha+1)} \to \infty$, we have

$$\sum_{i=a_n}^{b_n} \frac{z_{n,i}^{2\alpha}}{M_n} = \sum_{j=0}^{b_n - a_n} \frac{F(z_{n,a_n} + j/M_n)^2}{M_n} = \int_{1/2}^1 F(z)^2 \, dz + o(1) = \bigl(1 + o(1)\bigr) \int_{1/2}^1 z^{2\alpha} \, dz \tag{3.6.27}$$

as $n \to \infty$, by a Riemann sum approximation to the (uniformly) continuous function F on $[1/2, 1]$. Since $\bigl|\sum_{i=a_n}^{b_n} M_n^{-1} \,\tilde{\eta}_n(z_{n,i})\, z_{n,i}^{2\alpha}\bigr| \le \sup_{z \in [1/2,1]} |\tilde{\eta}_n(z)| \sum_{i=a_n}^{b_n} M_n^{-1} z_{n,i}^{2\alpha} = o(1)$, we deduce that

$$\|\widetilde{\theta}^{a_n,b_n}\|^2 = B^2 nu_n^{2\alpha+1} \bigl(1 + o(1)\bigr) \int_{1/2}^1 z^{2\alpha} \, dz. \tag{3.6.28}$$

For $\gamma \ge 0$, we can use the rescaled design points $z_{n,i}$ and argue as in (3.6.26) and (3.6.27) to see that

$$s_{n,\gamma} := \sum_{i=a_n}^{b_n} (x_i - m_0)^\gamma = nu_n^{\gamma+1} \sum_{i=a_n}^{b_n} \frac{z_{n,i}^\gamma}{M_n} = nu_n^{\gamma+1} \bigl(1 + o(1)\bigr) \int_{1/2}^1 z^\gamma \, dz$$

and

$$\begin{aligned}\tilde{s}_{n,\gamma} := \sum_{i=a_n}^{b_n} \bigl(1+\eta(x_i-m_0)\bigr)(x_i-m_0)^\gamma &= nu_n^{\gamma+1}\sum_{i=a_n}^{b_n} M_n^{-1}\bigl(1+\eta(u_n z_{n,i})\bigr)z_{n,i}^\gamma \\ &= nu_n^{\gamma+1}\bigl(1+o(1)\bigr)\int_{1/2}^1 z^\gamma\,dz;\end{aligned}$$

see also (3.6.19), (3.6.23) and (3.6.24) in the proof of Lemma 3.5.8. Now writing $x_i - \bar{x}_{a_n,b_n} = (x_i - m_0) - (\bar{x}_{a_n,b_n} - m_0)$ for $a_n \le i \le b_n$ and $\bar{x}_{a_n,b_n} - m_0 = s_{n,1}/s_{n,0}$, we have

$$\begin{aligned}\langle\widetilde{\theta}^{a_n,b_n},\mathbf{1}^{a_n,b_n}\rangle &= \textstyle\sum_{i=a_n}^{b_n} B\bigl(1+\eta(x_i-m_0)\bigr)(x_i-m_0)^\alpha = B\tilde{s}_{n\alpha}\\ \langle\widetilde{\theta}^{a_n,b_n},\widetilde{x}^{a_n,b_n}\rangle &= \textstyle\sum_{i=a_n}^{b_n} B\bigl(1+\eta(x_i-m_0)\bigr)(x_i-\bar{x}_{a_n,b_n})(x_i-m_0)^\alpha = B(\tilde{s}_{n,\alpha+1}-\tilde{s}_{n,\alpha}s_{n,1}/s_{n,0})\\ \|\mathbf{1}^{a_n,b_n}\|^2 &= \textstyle\sum_{i=a_n}^{b_n} 1 = s_{n,0}\\ \|\widetilde{x}^{a_n,b_n}\|^2 &= \textstyle\sum_{i=a_n}^{b_n}(x_i-\bar{x}_{a_n,b_n})^2 = \sum_{i=a_n}^{b_n}\{(x_i-m_0)^2-(\bar{x}_{a_n,b_n}-m_0)^2\} = s_{n,2}-s_{n,1}^2/s_{n,0}.\end{aligned}$$

Setting $\bar{z} := 3/4$, we note that $s_{n,1}/s_{n,0} = u_n\bigl(1+o(1)\bigr)\bar{z}$. Therefore, the second and third terms in (3.6.25) can be written as

$$\begin{aligned}c_{n0}^2\,\|\mathbf{1}^{a_n,b_n}\|^2 &= \frac{\langle\widetilde{\theta}^{a_n,b_n},\mathbf{1}^{a_n,b_n}\rangle^2}{\|\mathbf{1}^{a_n,b_n}\|^2} = \frac{B^2\tilde{s}_{n,\alpha}^2}{s_{n,0}} = B^2nu_n^{2\alpha+1}\bigl(1+o(1)\bigr)\left(\frac{\int_{1/2}^1 z^\alpha\,dz}{\int_{1/2}^1 dz}\right)^2\\ c_{n1}^2\,\|\widetilde{x}^{a_n,b_n}\|^2 &= \frac{\langle\widetilde{\theta}^{a_n,b_n},\widetilde{x}^{a_n,b_n}\rangle^2}{\|\widetilde{x}^{a_n,b_n}\|^2} = \frac{B^2(\tilde{s}_{n,\alpha+1}-\tilde{s}_{n,\alpha}s_{n,1}/s_{n,0})^2}{s_{n,2}-s_{n,1}^2/s_{n,0}}\\ &= B^2nu_n^{2\alpha+1}\bigl(1+o(1)\bigr)\left(\frac{\int_{1/2}^1(z-\bar{z})z^\alpha\,dz}{\int_{1/2}^1(z-\bar{z})^2\,dz}\right)^2. \qquad (3.6.29)\end{aligned}$$

Now for $G,\tilde{G}\in L^2[1/2,1]$, let $\langle G,\tilde{G}\rangle_* := \int_{1/2}^1 G(z)\,\tilde{G}(z)\,dz$ and $\|G\|_*^2 := \langle G,G\rangle_*$. Moreover, define $G_0,G_1\colon[1/2,1]\to\mathbb{R}$ by $G_0(z) := 1$ and $G_1(z) := z-\bar{z}$. These span the (closed) subspace $\mathcal{L}$ of affine functions $G\colon[1/2,1]\to\mathbb{R}$ and satisfy $\langle G_0,G_1\rangle_* = 0$. Let $c_j^* := \langle F,G_j\rangle_*/\|G_j\|_*^2$ for $j=0,1$, so that $F^* := c_0^*G_0 + c_1^*G_1$ is the projection of $F\colon z\mapsto z^\alpha$ onto $\mathcal{L}$ with respect to $\langle\cdot\,,\cdot\rangle_*$. Since $\alpha\neq 1$ in Assumption 2, we have $F\notin\mathcal{L}$, so

$$\rho_\alpha := \|F\|_*^2 - c_0^*\|G_0\|_*^2 - c_1^*\|G_1\|_*^2 = \|F-c_0^*G_0-c_1^*G_1\|_*^2 = \|F-F^*\|_*^2 = \textstyle\int_{1/2}^1(F-F^*)^2 > 0. \quad (3.6.30)$$

Thus, for all sufficiently large n, we can combine (3.6.25), (3.6.28), (3.6.29) and (3.6.30) to conclude that

$$\begin{aligned}\inf_{(a,b)\in\mathcal{T}_n}\inf_{c_0,c_1}\|\theta^{a,b}-c_0\mathbf{1}^{a,b}-c_1x^{a,b}\|^2 \ge R_n &= B^2nu_n^{2\alpha+1}\bigl(1+o(1)\bigr)\bigl(\|F\|_*^2 - c_0^*\|G_0\|_*^2 - c_1^*\|G_1\|_*^2\bigr)\\ &= \rho_\alpha B^2nu_n^{2\alpha+1}\bigl(1+o(1)\bigr).\end{aligned}$$

Since $u_n = 2^{-1}C_n(n/\log n)^{-1/(2\alpha+1)} = 2^{-1}C_n\bigl(1+o(1)\bigr)(n/\log n)^{-1/(2\alpha+1)}$ for all n, this completes the proof. □

Proof of Lemma 3.5.10. Let $h\in\mathcal{G}$ be such that $h(x_i) := \bigl(\theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'}\bigr)_{\tilde{k}\vee i\wedge\tilde{k}'}$ for $i\in[n]$. Since $x_{\tilde{k}}, x_{\tilde{k}'}$ are successive knots of $\hat{f}_n^{m_0}\in\mathcal{F}^{m_0}$ by assumption, $\breve{\theta}^{\tilde{k},\tilde{k}'} = \bigl(\hat{f}_n^{m_0}(x_{\tilde{k}}),\dots,\hat{f}_n^{m_0}(x_{\tilde{k}'})\bigr)$ is an affine sequence. Recalling that $f_0\in\mathcal{F}^{m_0}$ and $\theta^{\tilde{k},\tilde{k}'} = \bigl(f_0(x_{\tilde{k}}),\dots,f_0(x_{\tilde{k}'})\bigr)$, we can verify that $\hat{f}_n^{m_0}+\eta h\in\mathcal{H}^{m_0}$ for all sufficiently small $\eta>0$. Defining $\breve{\theta} := \bigl(\hat{f}_n^{m_0}(x_1),\dots,\hat{f}_n^{m_0}(x_n)\bigr)$,

$\theta := \big(f_0(x_1), \ldots, f_0(x_n)\big)$ and $Y^{\tilde{k},\tilde{k}'} := (Y_{\tilde{k}}, \ldots, Y_{\tilde{k}'})$, we deduce from (3.5.3) or Lemma 3.6.1 that

$$\begin{aligned} 0 &\geq \sum_{i=1}^{n} h(x_i)(Y_i - \breve{\theta}_i) \\ &= \big(\theta_{\tilde{k}} - \breve{\theta}_{\tilde{k}}\big) \sum_{i=1}^{\tilde{k}-1} (Y_i - \breve{\theta}_i) + \big\langle \theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'}, Y^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'} \big\rangle + \big(\theta_{\tilde{k}'} - \breve{\theta}_{\tilde{k}'}\big) \sum_{i=\tilde{k}'}^{n} (Y_i - \breve{\theta}_i). \end{aligned}$$

Now since $x_{\tilde{k}}, x_{\tilde{k}'}$ are knots of $\hat{f}_n^{m_0}$, it follows from (3.5.4) in the proof of Lemma 3.5.1 (specialised to the setting of Proposition 3.5.4) that

$$|\textstyle\sum_{i=1}^{\tilde{k}-1} (Y_i - \breve{\theta}_i)| \leq |Y_{\tilde{k}} - \breve{\theta}_{\tilde{k}}| \leq |\theta_{\tilde{k}} - \breve{\theta}_{\tilde{k}}| + |\xi_{\tilde{k}}| \quad \text{and} \quad |\textstyle\sum_{i=\tilde{k}'}^{n} (Y_i - \breve{\theta}_i)| \leq |Y_{\tilde{k}'} - \breve{\theta}_{\tilde{k}'}| \leq |\theta_{\tilde{k}'} - \breve{\theta}_{\tilde{k}'}| + |\xi_{\tilde{k}'}|.$$

Therefore, writing $Y^{\tilde{k},\tilde{k}'} = \theta^{\tilde{k},\tilde{k}'} + \xi^{\tilde{k},\tilde{k}'}$, we have

$$\|\theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'}\|^2 \leq \langle \xi^{\tilde{k},\tilde{k}'}, \breve{\theta}^{\tilde{k},\tilde{k}'} - \theta^{\tilde{k},\tilde{k}'} \rangle + |\theta_{\tilde{k}} - \breve{\theta}_{\tilde{k}}| \big(|\theta_{\tilde{k}} - \breve{\theta}_{\tilde{k}}| + |\xi_{\tilde{k}}|\big) + |\theta_{\tilde{k}'} - \breve{\theta}_{\tilde{k}'}| \big(|\theta_{\tilde{k}'} - \breve{\theta}_{\tilde{k}'}| + |\xi_{\tilde{k}'}|\big).$$

Since $|\theta_{\tilde{k}} - \breve{\theta}_{\tilde{k}}| \vee |\theta_{\tilde{k}'} - \breve{\theta}_{\tilde{k}'}| \leq \|\theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'}\|$, this implies that

$$\|\theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'}\| \leq \frac{\langle \xi^{\tilde{k},\tilde{k}'}, \breve{\theta}^{\tilde{k},\tilde{k}'} - \theta^{\tilde{k},\tilde{k}'} \rangle}{\|\theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'}\|} + |\xi_{\tilde{k}}| + |\xi_{\tilde{k}'}| + |\theta_{\tilde{k}} - \breve{\theta}_{\tilde{k}}| + |\theta_{\tilde{k}'} - \breve{\theta}_{\tilde{k}'}|.$$

Finally, $\breve{\theta}^{\tilde{k},\tilde{k}'}$ is an affine sequence belonging to $A_{\tilde{k},\tilde{k}'} = \operatorname{span}\{\mathbf{1}^{\tilde{k},\tilde{k}'}, x^{\tilde{k},\tilde{k}'}\}$, so $\theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'} \in L_{\tilde{k},\tilde{k}'} = \operatorname{span}\{\theta^{\tilde{k},\tilde{k}'}, \mathbf{1}^{\tilde{k},\tilde{k}'}, x^{\tilde{k},\tilde{k}'}\}$ and it follows as in (3.5.22) that

$$\frac{\langle \xi^{\tilde{k},\tilde{k}'}, \breve{\theta}^{\tilde{k},\tilde{k}'} - \theta^{\tilde{k},\tilde{k}'} \rangle}{\|\theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'}\|} \leq \|\Pi_{\tilde{k},\tilde{k}'}\, \xi^{\tilde{k},\tilde{k}'}\| \leq \max_{1 \leq a \leq b \leq n} \|\Pi_{a,b}\, \xi^{a,b}\|.$$

Since $|\theta_{\tilde{k}} - \breve{\theta}_{\tilde{k}}| + |\theta_{\tilde{k}'} - \breve{\theta}_{\tilde{k}'}| \leq 2 \max_{1 \leq i \leq n} |\theta_i - \breve{\theta}_i| = 2 \max_{1 \leq i \leq n} |(\hat{f}_n^{m_0} - f_0)(x_i)|$, we conclude that

$$\|\theta^{\tilde{k},\tilde{k}'} - \breve{\theta}^{\tilde{k},\tilde{k}'}\| \leq \max_{1 \leq a \leq b \leq n} \|\Pi_{a,b}\, \xi^{a,b}\| + 2 \max_{1 \leq i \leq n} |(\hat{f}_n^{m_0} - f_0)(x_i)| + 2 \max_{1 \leq i \leq n} |\xi_i| = \Xi,$$

as required. □

Proof of Lemma 3.5.11. For $\delta \in (0, (1 - m_0)/2]$ and $t \in [0, (1 - m_0)/\delta]$, let

$$g_{0,\delta}(t) := \delta^{-\alpha}\big(f_0(m_0) + f_0'(m_0)\delta t - f_0(m_0 + \delta t)\big) \quad \text{and} \quad u_\delta := \delta^{-(\alpha-1)}\big(f_0'(m_0) - u(m_0 + \delta)\big),$$

where $\alpha > 1$. Then $g_{0,\delta}$ is convex and non-negative on $[0, 2]$ for each such δ, and since $u(m_0 + \delta)$ was taken to be a subgradient of $f_0|_{[m_0,1]}$ at $m_0 + \delta$, we see that u_δ is a subgradient of $g_{0,\delta}$ at $t = 1$. Assumption 2 ensures that $g_{0,\delta}$ converges uniformly on $[0, 2]$ to the function $g_0 \colon t \mapsto Bt^\alpha$ as $\delta \to 0$, and so by taking $C = (0, 2)$ in Seijo and Sen (2011, Lemma 3.10), we deduce further that $u_\delta \to g_0'(1) = B\alpha$ as $\delta \to 0$.

Moreover, for $\delta \in (0, (1 - m_0)/2]$ and $t \in [0, 1]$, let

$$\begin{aligned} g_{1,\delta}(t) &:= \delta^{-\alpha}\big(f_0(m_0) + f_0'(m_0)\delta t - f_{1,\delta}(m_0 + \delta t)\big) \\ &= \delta^{-\alpha}\big\{\big(f_0(m_0) + f_0'(m_0)\delta - f_0(m_0 + \delta)\big) - \delta(1 - t)\big(f_0'(m_0) - u(m_0 + \delta)\big)\big\} \\ &= g_{0,\delta}(1) - (1 - t)u_\delta \leq g_{0,\delta}(t) \\ \text{and} \qquad g_{2,\delta}(t) &:= \delta^{-\alpha}\big(f_0(m_0) + f_0'(m_0)\delta t - f_{2,\delta}(m_0 + \delta t)\big) = -\delta t^\alpha, \end{aligned}$$

where $f_{1,\delta}, f_{2,\delta}$ are as defined in the proof of Proposition 3.3.4. Recalling from (3.5.36) that $f_\delta = f_{1,\delta} \wedge f_{2,\delta}$ on $[m_0, m_0 + \delta]$ by definition, we have

$$g_\delta(t) := \delta^{-\alpha}\bigl(f_0(m_0) + f_0'(m_0)\delta t - f_\delta(m_0 + \delta t)\bigr) = g_{1,\delta}(t) \vee g_{2,\delta}(t) \tag{3.6.31}$$

for all $t \in [0,1]$. Note that $g_{1,\delta}(0) < g_{0,\delta}(0) = 0 \leq g_{2,\delta}(0)$ and $g_{1,\delta}(1) = g_{0,\delta}(1) \geq 0 > g_{2,\delta}(1)$. Thus, since $g_{1,\delta}, g_{2,\delta}$ are continuous functions that are strictly increasing and strictly decreasing respectively, there is a unique $c_\delta \in (0,1)$ satisfying $g_{1,\delta} \leq g_{2,\delta}$ on $[0, c_\delta]$ and $g_{1,\delta} \geq g_{2,\delta}$ on $[c_\delta, 1]$; in other words, $f_{1,\delta} \geq f_{2,\delta}$ on $[m_0, m_0 + \delta c_\delta]$ and $f_{1,\delta} \leq f_{2,\delta}$ on $[m_0 + \delta c_\delta, m_0 + \delta]$, so this is consistent with the definition of c_δ in the proof of Proposition 3.3.4. Since $g_{0,\delta}(1) - (1 - c_\delta)u_\delta = g_{1,\delta}(c_\delta) = g_{2,\delta}(c_\delta) \in [-\delta, 0]$, we have

$$1 - u_\delta^{-1} g_{0,\delta}(1) \geq c_\delta \geq 1 - u_\delta^{-1}\bigl(g_{0,\delta}(1) + \delta\bigr).$$

In the limit as $\delta \to 0$, it was shown above that $g_{0,\delta}(1) \to g_0(1) = B$ and $u_\delta \to g_0'(1) = B\alpha$, so $c_\delta \to 1 - \alpha^{-1}$ and $g_{1,\delta}$ converges uniformly on $[0,1]$ to the affine function $g_1 : t \mapsto g_0(1) - (1-t)g_0'(1) = B\bigl(1 - (1-t)\alpha\bigr)$. Consequently, $g_\delta = g_{1,\delta} \vee g_{2,\delta} \to g_1 \vee 0 \equiv g_1^+$ uniformly on $[0,1]$ as $\delta \to 0$.

Now let (δ_n) be any sequence such that $\delta_n \to 0$ and $n\delta_n \to 0$ as $n \to \infty$. Having already shown that $\lim_{n\to\infty} c_{\delta_n} = 1 - \alpha^{-1}$, we proceed to establish the claimed limiting expression for $\|f_{\delta_n} - f_0\|_n^2$. For each n, let $z_{n,i} := (x_i - m_0)/\delta_n$ for $i \in [n]$, where $x_i \equiv x_{ni} = i/n$ by Assumption 2, so that $z_{n,i+1} - z_{n,i} = 1/(n\delta_n)$ for all $i \in [n-1]$. Then recalling from (3.5.36) that $f_{\delta_n} = f_0$ on $[0,1] \setminus (m_0, m_0 + \delta_n)$, we can use (3.6.31) to write

$$\|f_{\delta_n} - f_0\|_n^2 = \frac{1}{n} \sum_{i\,:\, m_0 < x_i < m_0 + \delta_n} (f_{\delta_n} - f_0)^2(x_i) = \delta_n^{2\alpha+1} \frac{1}{n\delta_n} \sum_{i\,:\,0 < z_{n,i} < 1} (g_{\delta_n} - g_{0,\delta_n})^2(z_{n,i}) \tag{3.6.32}$$

for each n. Since $|\{i : 0 < z_{n,i} < 1\}| = O(n\delta_n)$ and $(g_{\delta_n} - g_{0,\delta_n})^2 \to (g_1^+ - g_0)^2$ uniformly on $[0,1]$ as $n \to \infty$, we have

$$\begin{aligned}
&\frac{1}{n\delta_n} \sum_{i\,:\,0 < z_{n,i} < 1} \bigl|(g_{\delta_n} - g_{0,\delta_n})^2(z_{n,i}) - (g_1^+ - g_0)^2(z_{n,i})\bigr| \\
&\qquad\qquad \leq \frac{|\{i : 0 < z_{n,i} < 1\}|}{n\delta_n} \sup_{x \in [0,1]} \bigl|(g_{\delta_n} - g_{0,\delta_n})^2 - (g_1^+ - g_0)^2\bigr| = o(1).
\end{aligned}$$

Thus, by a Riemann sum approximation to the (uniformly) continuous function $(g_1^+ - g_0)^2$ on $[0,1]$ and the fact that $n\delta_n \to \infty$, we see that

$$\begin{aligned}
\frac{1}{n\delta_n} \sum_{i\,:\,0 < z_{n,i} < 1} (g_{\delta_n} - g_{0,\delta_n})^2(z_{n,i}) &= \frac{1}{n\delta_n} \sum_{i\,:\,0 < z_{n,i} < 1} (g_1^+ - g_0)^2(z_{n,i}) + o(1) \\
&= \int_0^1 (g_1^+ - g_0)^2 + o(1) \\
&= B^2 \int_0^1 \bigl\{t^\alpha - \bigl(1 - (1-t)\alpha\bigr)^+\bigr\}^2\, dt + o(1) \\
&= \bigl(1 + o(1)\bigr) C_\alpha B^2
\end{aligned}$$

as $n \to \infty$, where $C_\alpha := \int_0^1 \bigl\{t^\alpha - \bigl(1 - (1-t)\alpha\bigr)^+\bigr\}^2\, dt$. Combining this with (3.6.32) yields the desired conclusion. □

3.6.3 Proofs for Section 3.5.4

Proof of Proposition 3.5.12. (a) Since every $g \in \mathcal{F}^m$ is bounded on $[0,1]$, it follows that $\mathcal{F}^m \subseteq L^2(\nu)$. If $g, h \in \mathcal{F}^m$, then certainly $\lambda g \in \mathcal{F}^m$ for all $\lambda > 0$ and $\lambda g + (1-\lambda)h \in \mathcal{F}^m$ for all $\lambda \in [0,1]$. Now fix $g \in \mathcal{F}^m$, and for each $n \in \mathbb{N}$, let $g_n \colon [0,1] \to \mathbb{R}$ be the Lipschitz function that agrees with g on $[0, m(1-1/n)] \cup \{m\} \cup [m(1-1/n)+1/n, 1]$, and is also linear on both $[m(1-1/n), m]$ and $[m, m(1-1/n)+1/n]$. Then $g_n \in \mathcal{F}^m$ and $g(0) \leq g_n \leq g(1)$ for all n, and since $g_n \to g$ pointwise, we have $\|g_n - g\|_{L^2(\nu)} \to 0$ by the dominated convergence theorem.

(b) Let $M_\nu^L := \min(\operatorname{supp}\nu)$ and $M_\nu^R := \max(\operatorname{supp}\nu)$, so that $\operatorname{csupp}\nu = [M_\nu^L, M_\nu^R]$. There is nothing to prove when $m \in \operatorname{csupp}\nu$, so suppose now that $m > M_\nu^R$. Then $\tilde{m} = M_\nu^R$, and note that $g \colon [0,\tilde{m}] \to \mathbb{R}$ is increasing, convex and Lipschitz if and only if there exists a Lipschitz $f \in \mathcal{F}^m$ such that $g = f|_{[0,\tilde{m}]}$. Thus, $\mathcal{F}_\nu^m = \{[f]_\nu : f \in \mathcal{F}^{\tilde{m}} \text{ is Lipschitz}\}$ is dense in $\mathcal{F}_\nu^{\tilde{m}}$ by (a). The case $m < M_\nu^L$ is similar.

(c, $\Leftarrow$) We first show that if $(f_n)_{n=1}^\infty$ is a sequence of functions in $\mathcal{F}^m$ such that $\|f_n - f\|_{L^2(\nu)} \to 0$ for some $f \in L^2(\nu)$, then under any one of the conditions (i)–(iii) above, there exists $g \in \mathcal{F}^m$ such that $f \sim_\nu g$. To begin with, note that $f_n \to f$ in ν-measure, so there exists a subsequence $(g_k)_{k=1}^\infty \equiv (f_{n_k})_{k=1}^\infty$ such that $g_k \to f$ ν-almost everywhere. In each of the cases below, we will in fact show that there is some $g \in \mathcal{F}^m$ that agrees with f on $A := \{x \in \operatorname{supp}\nu : g_k(x) \to f(x)\}$, which is a dense subset of $\operatorname{supp}\nu$. Indeed, if $S \subseteq \operatorname{supp}\nu$ satisfies $\nu(S^c \cap \operatorname{supp}\nu) = 0$, then by the definition of $\operatorname{supp}\nu$, the set $S^c \cap \operatorname{supp}\nu$ has empty interior; in other words, S is dense in $\operatorname{supp}\nu$.

Case 1 – $\nu([0,m)) \wedge \nu((m,1]) > 0$: Since A is dense in $\operatorname{supp}\nu$, there exist $a_L, a_R \in A \subseteq \operatorname{supp}\nu$ such that $a_L < m < a_R$ and $g_k \to f$ on $\{a_L, a_R\}$. Since the functions g_k are convex on $[0,m]$, concave on $[m,1]$ and increasing on $[0,1]$, we have

$$\begin{aligned}
\liminf_{k\to\infty} g_k(0) &\geq \liminf_{k\to\infty} \frac{m\, g_k(a_L) - a_L\, g_k(m)}{m - a_L} \geq \frac{m\, f(a_L) - a_L\, f(a_R)}{m - a_L} \\
\limsup_{k\to\infty} g_k(1) &\leq \limsup_{k\to\infty} \frac{(1-m)\, g_k(a_R) - (1-a_R)\, g_k(m)}{a_R - m} \leq \frac{(1-m)\, f(a_R) - (1-a_R)\, f(a_L)}{a_R - m},
\end{aligned} \tag{3.6.33}$$

so $\{g_k(x)\}_{k=1}^\infty$ is bounded for each $x \in [0,1]$. Therefore, by considering separately the intervals $(0,m), (m,1)$, we can apply Rockafellar (1997, Theorem 10.9) and extract a subsequence (g_{k_ℓ}) of (g_k) that converges pointwise on $(0,m) \cup (m,1)$. In fact, (g_{k_ℓ}) converges pointwise on $[0,1] \setminus \{m\}$ by Lemma 3.6.12, and the limit function g is convex on $[0,m)$, concave on $(m,1]$ and increasing on $[0,1] \setminus \{m\}$. If in addition $m \in A$, then

$$g(z) = \lim_{\ell\to\infty} g_{k_\ell}(z) \leq \lim_{\ell\to\infty} g_{k_\ell}(m) = f(m) \leq \lim_{\ell\to\infty} g_{k_\ell}(w) = g(w)$$

for all $z \in (0,m)$ and $w \in (m,1)$, so $\lim_{x \nearrow m} g(x) \leq f(m) \leq \lim_{x \searrow m} g(x)$. Thus, we can extend g to a function on $[0,1]$ that belongs to $\mathcal{F}^m$ by setting $g(m) = f(m)$. Otherwise, if $m \notin A$, then we can set $g(m) = \lim_{x \searrow m} g(x)$ for concreteness. In both cases, we have $g \in \mathcal{F}^m$ and $f = g$ on A, as required.

Case 2 – $\nu((m,1]) = 0$: Here, we have $\operatorname{supp}\nu \subseteq [0,m]$. We also assume that $\operatorname{supp}\nu$ contains at least two points, since otherwise the result holds trivially. Note that $\operatorname{conv}(\operatorname{Cl} A) \supseteq \operatorname{Int}\operatorname{csupp}\nu = (M_\nu^L, M_\nu^R)$. By convexity arguments similar to those given in Case 1, it follows that $\{g_k(x)\}_{k=1}^\infty$ is bounded for all $x \in (M_\nu^L, M_\nu^R)$. Thus, again by Rockafellar (1997, Theorem 10.9) and Lemma 3.6.12, there exists a subsequence (g_{k_ℓ}) of (g_k) that converges pointwise on $[0, M_\nu^R)$ to some increasing convex function $g \colon [0, M_\nu^R) \to \mathbb{R}$. By the definition of A, we must have $f = g$ on $[0, M_\nu^R) \cap A$.

- If condition (i) holds, then $M_\nu^R = m$ and $\nu(\{m\}) > 0$, so $m \in A$, i.e. $g_k(m) \to f(m)$. We now extend g to $[0,1]$ by setting $g(x) = f(m)$ for all $x \in [m,1]$. Then $f = g$ on A, and for all $x \in [0,m)$, we have $g(x) = \lim_{\ell\to\infty} g_{k_\ell}(x) \leq \lim_{\ell\to\infty} g_{k_\ell}(m) = f(m)$, so $g \in \mathcal{F}^m$.

- If condition (ii) holds, then $M_\nu^R \in (0,m)$ is an isolated point of $\operatorname{supp}\nu$, so $\nu(\{M_\nu^R\}) > 0$, $M_\nu^R \in A$ and $M_\nu' := \max(\operatorname{supp}\nu \setminus \{M_\nu^R\}) < M_\nu^R < m$. Let $h\colon [0,1] \to \mathbb{R}$ be the function that agrees with f on $[0, M_\nu'] \cup \{M_\nu^R\}$ and is linear on $[M_\nu', 1]$. Then h is linear on $[m,1]$ and convex and increasing on $[0,1]$, so $h \in \mathcal{F}^m$. Since $(M_\nu', 1] \cap A = \{M_\nu^R\}$, the functions f, g, h agree on A, as required.

The analogous case where $\operatorname{supp}\nu \subseteq [m,1]$ can be handled in much the same way, and so we have now demonstrated the sufficiency of each of the conditions (i), (ii) and (iii).

(c, $\Rightarrow$) Supposing that none of the conditions (i)–(iii) hold, we now verify that $\operatorname{Cl}\mathcal{F}_\nu^m \supsetneqq \mathcal{F}_\nu^m$. We consider only the cases where $\operatorname{supp}\nu \subseteq [0,m]$; the arguments are similar if $\operatorname{supp}\nu \subseteq [m,1]$.

Case 1 – $\nu(\{M_\nu^R\}) = 0$: Note that there exists $f \in L^2(\nu)$ such that $f|_{E_\nu}$ is convex and increasing, and $f(x) \to \infty$ as $x \nearrow M_\nu^R$. Indeed, a concrete example of such a function can be obtained via the following construction: since M_ν^R is not an isolated point of $\operatorname{supp}\nu$ by assumption, there exists a sequence $(a_n \in \operatorname{supp}\nu \setminus \{M_\nu^R\} : n \in \mathbb{N})$ such that $a_n \nearrow M_\nu^R$ and $\nu((a_n, M_\nu^R)) \leq 2^{-3n}$ for all n. For each n, let $h_n\colon [0,1] \to \mathbb{R}$ be such that $h_n = 0$ on $[0, a_n]$, $h_n(M_\nu^R) = 2^{n/2}$ and h_n is linear on $[a_n, 1]$. Then h_n is convex and increasing, and $\|h_n\|_{L^2(\nu)} \leq (2^n \cdot 2^{-3n})^{1/2} = 2^{-n}$. Thus, the function $h\colon [0,1] \to \mathbb{R}$ defined by $h(x) := \sum_{n=1}^\infty h_n(x)\mathbb{1}_{\{x<M_\nu^R\}}$ is also convex and increasing. Moreover, $\|h\|_{L^2(\nu)} \leq \sum_{n=1}^\infty \|h_n\|_{L^2(\nu)} < \infty$ and $h(x) \to \infty$ as $x \nearrow M_\nu^R$.

For any f with the above properties, we now argue that $[f]_\nu \notin \mathcal{F}_\nu^m$, i.e. that there does not exist $g \in \mathcal{F}^m$ such that $f \sim_\nu g$. Indeed, if g is a function that agrees with f on a set $S \subseteq \operatorname{supp}\nu$ with the property that $\nu(S^c \cap \operatorname{supp}\nu) = 0$, then recall from the second paragraph of the proof that S is dense in $\operatorname{supp}\nu$. Thus, since M_ν^R is not an isolated point of $\operatorname{supp}\nu$, there exists a sequence $(s_n \in S \setminus \{M_\nu^R\} : n \in \mathbb{N})$ such that $s_n \to M_\nu^R$, and we must have $g(s_n) = f(s_n)$ for all n. But this implies that $g(x) \to \infty$ as $x \nearrow M_\nu^R$, so g cannot be extended to a finite convex function on $[0,m]$.

Case 2 – $\nu(\{M_\nu^R\}) > 0$: Consider any $f \in L^2(\nu)$ such that $f|_{E_\nu}$ is convex and increasing, and f is discontinuous at M_ν^R. Since $M_\nu^R \in (0,m)$ is not an isolated point of $\operatorname{supp}\nu$, we deduce as before that if $f \sim_\nu g$ for some $g\colon [0,1] \to \mathbb{R}$, then there exists a sequence $(s_n \in \operatorname{supp}\nu \setminus \{M_\nu^R\} : n \in \mathbb{N})$ such that $s_n \to M_\nu^R$ and $g(s_n) = f(s_n)$ for all n. But since $\nu(\{M_\nu^R\}) > 0$, we have $g(M_\nu^R) = f(M_\nu^R) \neq \lim_{n\to\infty} f(s_n) = \lim_{n\to\infty} g(s_n)$, so g is not continuous at $M_\nu^R \in (0,m)$ and hence does not belong to $\mathcal{F}^m$. This shows that $[f]_\nu \notin \mathcal{F}_\nu^m$ and hence that $\operatorname{Cl}\mathcal{F}_\nu^m \supsetneqq \mathcal{F}_\nu^m$, as required.

(d) Suppose again that none of the conditions (i)–(iii) hold, assuming for the time being that $\operatorname{supp}\nu \subseteq [0,m]$. Then $m > 0$ and $M_\nu^R \in [0,m]$ is not an isolated point of $\operatorname{supp}\nu$. Let $(f_n)_{n=1}^\infty$ be any sequence in $\mathcal{F}^m$ such that $\|f_n - f\|_{L^2(\nu)} \to 0$ for some $f \in L^2(\nu)$. By a very similar argument to that given in the first bullet point in Case 2 of (c, $\Leftarrow$), there exists an increasing convex g defined on E_ν that agrees ν-almost everywhere with f; recall that E_ν contains M_ν^R if and only if $\nu(\{M_\nu^R\}) > 0$. Since $\mathcal{F}_\nu^m = \{[f]_\nu : f \in \mathcal{F}^m\} \subseteq \mathcal{L}^2(\nu)$ by (a), we deduce that

$$\operatorname{Cl}\mathcal{F}_\nu^m \subseteq \{[f]_\nu : f \in L^2(\nu) \text{ and } f|_{E_\nu} \text{ is convex and increasing}\}.$$

For the reverse inclusion, we split into the two cases considered in (c, $\Rightarrow$) above.

Case 1 – $\nu(\{M_\nu^R\}) = 0$: Here, we have $M_\nu^R \notin E_\nu$. For a fixed $f \in L^2(\nu)$ such that $f|_{E_\nu}$ is convex and increasing, we claim that there exists a sequence $(f_n)_{n=1}^\infty$ in $\mathcal{F}^m$ such that $\|f_n - f\|_{L^2(\nu)} \to 0$. Indeed, fix a sequence $(x_n \in \operatorname{supp}\nu \setminus \{M_\nu^R\} : n \in \mathbb{N})$ such that $x_n \nearrow M_\nu^R$, and for each n, observe that since $f|_{E_\nu}$ has a finite and non-negative subgradient at x_n, there exists an increasing convex $f_n \in \mathcal{F}^m$ such that $f_n = f$ on $E_\nu \cap [0, x_n]$, f_n is linear on $[x_n, 1]$ and $f_n \leq f$ on E_ν. Thus, since

$\nu(E_\nu) = 1$, $\inf_{E_\nu} f \leq f_n \leq \sup_{E_\nu} f$ on E_ν for all n and $f_n \to f$ pointwise on E_ν, it follows by the dominated convergence theorem that $\|f_n - f\|^2_{L^2(\nu)} = \int_{E_\nu} |f_n - f|^2 \to 0$, as required.

Case 2 – $\nu(\{M^R_\nu\}) > 0$: Note that $M^R_\nu < m$ and $M^R_\nu \in E_\nu$ in this case. As before, take any $f \in L^2(\nu)$ such that $f|_{E_\nu}$ is convex and increasing, and fix a sequence $(x_n \in \operatorname{supp}\nu \setminus \{M^R_\nu\} : n \in \mathbb{N})$ such that $x_n \nearrow M^R_\nu$. For each n, let f_n be the (unique) function that satisfies $f_n = f$ on $[0, x_n] \cup \{M^R_\nu\}$ and is linear on $[x_n, 1]$. Then $f_n \in \mathcal{F}^m$ for all n by the convexity of f, and $f_n \to f$ pointwise on E_ν. Thus, since $\inf_{E_\nu} f \leq f_n \leq f(M^R_\nu) < \infty$ on E_ν for all n, we can once again apply the dominated convergence theorem to deduce that $\|f_n - f\|^2_{L^2(\nu)} = \int_{E_\nu} |f_n - f|^2 \to 0$. This shows that $\operatorname{Cl}\mathcal{F}^m_\nu \supseteq \{[f]_\nu : f \in L^2(\nu) \text{ and } f|_{E_\nu} \text{ is convex and increasing}\}$ in this case.

Straightforward modifications of the arguments above yield the analogous conclusion when $\operatorname{supp}\nu \subseteq [m, 1]$. This completes the proof. □

Proof of Corollary 3.5.13. (a) For $f \in L^2(P^X)$, it is immediate from (3.5.38) that $f \in \psi^*_m(P)$ if and only if $[f]_{P^X} \in \mathcal{L}^2(P^X)$ is the projection of $[f_P]_{P^X}$ onto $\operatorname{Cl}\mathcal{F}^m_{P^X}$, which is a closed, convex subset of the Hilbert space $\mathcal{L}^2(P^X)$ by Proposition 3.5.12.

(b) This follows directly from the definition of $\psi^*_m(P)$ and the fact that every $f \in \mathcal{F}^m$ is bounded on $[0, 1]$.

(c) Since $\operatorname{Cl}\mathcal{F}^m_{P^X} = \operatorname{Cl}\mathcal{F}^{\tilde{m}}_{P^X}$ by Proposition 3.5.12(b), we have $\psi^*_m(P) = \psi^*_{\tilde{m}}(P)$ by definition, and $L^*_m(P) = L^*_{\tilde{m}}(P)$ by the observation after (3.5.38). If there exists $f \in \psi^0_m(P)$, then setting $\tilde{f}(x) := f(M_L \vee x \wedge M_R)$ for $x \in [0, 1]$ with $M_L := \min(\operatorname{supp} P^X)$ and $M_R := \max(\operatorname{supp} P^X)$, we have $\tilde{f} \in \psi^0_{\tilde{m}}(P)$.

(d) If condition (i) holds, then $\mathcal{F}^m_{P^X} = \operatorname{Cl}\mathcal{F}^m_{P^X}$ by Proposition 3.5.12(c). Thus, there exists $f^* \in \mathcal{F}^m$ such that $\psi^*(P) = [f^*]_{P^X}$ by (a) above, whence $f^* \in \psi^0_m(P)$.

Suppose now that condition (ii) holds, in which case $m = \tilde{m}$ and there exist a regression function f_P for P and $b, \varepsilon > 0$ such that $|f_P| \leq b$ on $(m - \varepsilon, m + \varepsilon)$. We may assume without loss of generality that $m = \max(\operatorname{supp} P^X)$; the case $m = \min(\operatorname{supp} P^X)$ is similar. Suppose for a contradiction that $\psi^0_m(P) = \emptyset$, i.e. that $\psi^*(P) \in \big(\operatorname{Cl}\mathcal{F}^m_{P^X}\big) \setminus \mathcal{F}^m_{P^X}$. In view of condition (i) in Proposition 3.5.12(c), this can only happen if $P^X(\{m\}) = 0$. By Proposition 3.5.12(d), we can write $\psi^*_m(P) = [f]_{P^X}$ for some $f \in L^2(P^X)$ that is convex and increasing on $\operatorname{Int}(\operatorname{csupp} P^X)$. Since $[f]_{P^X} = \psi^*_m(P) \notin \mathcal{F}^m_{P^X}$, the function $f|_{\operatorname{Int}(\operatorname{csupp} P^X)}$ cannot be extended to an element of $\mathcal{F}^m$, so we must have $f(x) \to \infty$ as $x \nearrow m$.

Therefore, we can find $m' \in \operatorname{Int}(\operatorname{csupp} P^X) \cap (m - \varepsilon, m)$ such that $f(x) > b$ for all $x \in [m', m)$. Since $f|_{\operatorname{Int}(\operatorname{csupp} P^X)}$ has a finite and non-negative subgradient at m', there exists an increasing convex $\tilde{f} \in \mathcal{F}^m$ such that $\tilde{f} = f$ on $\operatorname{Int}(\operatorname{csupp} P^X) \cap [0, m']$, $\tilde{f}$ is linear on $[m', 1]$ and $f_P \leq b < \tilde{f} \leq f$ on $[m', m)$. But this means that $\|\tilde{f} - f_P\|_{L^2(P^X)} < \|f - f_P\|_{L^2(P^X)}$, so $L^*_m(P) \leq L(\tilde{f}, P) < L(f, P)$ by (3.5.38), contradicting the fact that $f \in \psi^*_m(P)$. Thus, $\psi^*_m(P) \in \mathcal{F}^m_{P^X}$, whence $\psi^0_m(P) \neq \emptyset$.

(e) If $f, g \in \psi^0_m(P)$, then $f \sim_{P^X} g$ by (a), so $f = g$ on some dense subset $S \subseteq \operatorname{supp} P^X$; see the first paragraph of the proof of Proposition 3.5.12(c). It follows that $f = g$ on $(\operatorname{supp} P^X) \setminus \{m\}$, a set on which both f, g are continuous. If f, g are both continuous on $[0, 1]$, then $f = g$ on $\operatorname{supp} P^X$ by the same argument. If in addition $P^X(\{m\}) > 0$, then clearly $f(m) = g(m)$.

(f) The forward implication was established in (e). For the converse, suppose that $m \in \operatorname{supp} P^X$ and there is some $f \in \psi^0_m(P)$ that is discontinuous at m, so that $\lim_{x \nearrow m} f(x) < \lim_{x \searrow m} f(x)$. If $P^X(\{m\}) = 0$, then any $\psi^0_m(P)$ contains any $\tilde{f} \colon [0, 1] \to \mathbb{R}$ such that $\tilde{f} = f$ on $[0, 1] \setminus \{m\}$ and $\lim_{x \nearrow m} f(x) \leq \tilde{f}(m) \leq \lim_{x \searrow m} f(x)$, so the elements of $\psi^0_m(P)$ do not all agree at $m \in \operatorname{supp} P^X$.

(g) Suppose that $\psi^0_m(P)$ contains a continuous function $h \in \mathcal{F}^m$. For any other $f \in \psi^0_m(P)$, we know from (e) that $f = h$ on $(\operatorname{supp} P^X) \setminus \{m\}$. In view of the continuity of h at m and the assumption that $\operatorname{supp} P^X$ has non-empty intersection with both $(m - \varepsilon, m)$ and $(m, m + \varepsilon)$ for all $\varepsilon > 0$, this forces $f(m) = h(m)$, so $f = h$ on $\operatorname{supp} P^X$ and f is continuous. □

The proof of Proposition 3.5.14 relies on the following three key lemmas. Let the marginal distribution P^X on $[0,1]$ be as in Proposition 3.5.14, and define $M_L := \min(\operatorname{supp} P^X)$, $M_R := \max(\operatorname{supp} P^X)$ and $C := [M_L, M_R] = \operatorname{csupp} P^X$.

Lemma 3.6.9. *Fix $x \in \operatorname{Int} C$ and $\ell \in [0,\infty)$. Let (P_n) be a sequence in $\mathcal{P}$ that converges weakly to some $P \in \mathcal{P}$. Then there exists $B \equiv B(x,\ell,P) < \infty$ such that for any sequence of increasing functions $f_n\colon [0,1] \to \mathbb{R}$ with $\limsup_{n\to\infty} L(f_n,P_n) \le \ell$ for all n, we have $\limsup_{n\to\infty} |f_n(x)| < B$.*

Proof. Since $x \in \operatorname{Int} C$, we have $P^X([0,x)) \wedge P^X((x,1]) > 0$. Let (f_n) be as above. Then for each n, note that since f_n is increasing, we have

$$L(f_n,P_n) \ge \int_{[x,1]\times\mathbb{R}} \bigl(y - f_n(x)\bigr)^2 \, dP_n(x,y) \ge \left(\frac{f_n^+(x)}{2}\right)^2 P_n\left([x,1] \times \left(-\infty, \frac{f_n^+(x)}{2}\right]\right); \quad (3.6.34)$$

indeed, if $f_n(x) \le 0$, then (3.6.34) holds trivially, and if $f_n(x) > 0$, then for all $x' \in [x,1]$ and $y' \le f_n(x)/2$, we have $f_n(x') - y' \ge f_n(x) - y' \ge f_n(x)/2 > 0$.

Now let (f_{n_k}) be a subsequence such that $f_{n_k}^+(x) \to \limsup_{n\to\infty} f_n^+(x) =: 2s$ as $k \to \infty$. Since $P_n \xrightarrow{d} P$, an application of the portmanteau lemma (van der Vaart, 1998, Lemma 2.2) shows that

$$\liminf_{k\to\infty} \left(\frac{f_{n_k}^+(x)}{2}\right)^2 P_{n_k}\left((x,1] \times \left(-\infty, \frac{f_{n_k}^+(x)}{2}\right)\right) \ge s^2\, P\bigl((x,1] \times (-\infty,s)\bigr).$$

It follows from this and (3.6.34) that $s^2\, P\bigl((x,1] \times (-\infty,s)\bigr) \le \limsup_{n\to\infty} L(f_n,P_n) \le \ell$. Since $P\bigl((x,1] \times (-\infty,b)\bigr) \to P^X((x,1]) > 0$ as $b \to \infty$, we can therefore find $B' \equiv B'(x,\ell,P) < \infty$ such that $\limsup_{n\to\infty} f_n^+(x) = 2s < B'$ for any sequence (f_n) satisfying the conditions of Lemma 3.6.9. An analogous argument yields the same conclusion for $\limsup_{n\to\infty} f_n^-(x)$. $\square$

For sequences of S-shaped functions, the conclusion of Lemma 3.6.9 can be strengthened.

Lemma 3.6.10. *Fix $\ell \in [0,\infty)$ and let (m_n) be a sequence in $[0,1]$ that converges to some fixed $m_0 \in \operatorname{Int} C$. Then under the hypotheses of Lemma 3.6.9, there exists $\tilde{B} \equiv \tilde{B}(m_0,\ell,P) < \infty$ such that for any sequence (f_n) with $f_n \in \mathcal{F}^{m_n}$ for all n and $\limsup_{n\to\infty} L(f_n,P_n) \le \ell$, we have $\limsup_{n\to\infty} \sup_{x\in[0,1]} |f_n(x)| < \tilde{B}$.*

Proof. Since $m_n \to m_0 \in \operatorname{Int} C$, we can find $a_L, a_R \in \operatorname{Int} C$ such that $0 < a_L < m_0 < a_R < 1$, so that for all sufficiently large $n \in \mathbb{N}$, we have $f_n(a_L) \le f_n(m_n) \le f_n(a_R)$ and

$$\frac{m_n f_n(a_L) - a_L f_n(m_n)}{m_n - a_L} \le f_n(0) \le f_n(x) \le f_n(1) \le \frac{(1-m_n) f_n(m_n) - (1-a_R) f_n(a_L)}{a_R - m_n} \quad (3.6.35)$$

for all $x \in [0,1]$. Since $\limsup_{n\to\infty} L(f_n,P_n) \le \ell$, we have $\limsup_{n\to\infty} |f_n(x)| \le B(x,\ell,P) < \infty$ for $x \in \{a_L, a_R\}$ by Lemma 3.6.9, so the result follows from (3.6.35) and the fact that $m_n \to m_0$. $\square$

Another important consequence of Lemma 3.6.9 is the following. Recall that $\tilde{m}_0 = \operatorname{argmin}_{x\in C} |x - m_0|$.

Lemma 3.6.11. *Under the hypotheses of Proposition 3.5.14, let $(f_n)_{n=1}^\infty$ be any sequence with $f_n \in \mathcal{F}^{m_n}$ and $\limsup_{n\to\infty} L(f_n,P_n) < \infty$ for all n. Then for every subsequence $(g_k)_{k=1}^\infty \equiv (f_{n_k})_{k=1}^\infty$, there is a further subsequence (g_{k_ℓ}) and a function g defined on $[0,1]$ with the following properties:*

(i) g is increasing on $C \setminus \{\tilde{m}_0\}$, convex on $C \cap [0,\tilde{m}_0)$ and concave on $C \cap (\tilde{m}_0, 1]$.

(ii) $g_{k_\ell} \to g$ pointwise on C and uniformly on closed subsets of $C \setminus \{\tilde{m}_0\}$. In particular, if $z_\ell \to z \in C \setminus \{\tilde{m}_0\}$, then $g_{k_\ell}(z_\ell) \to g(z)$.

(iii) $g(x) \in \mathbb{R}$ *for all* $x \in C \setminus \{\tilde{m}_0\}$*, and* $g(\tilde{m}_0) \in (-\infty, \infty]$ *if* $\tilde{m}_0 > M_L$ *and* $g(\tilde{m}_0) \in [-\infty, \infty)$ *if* $\tilde{m}_0 < M_R$*.*

(iv) $g \in \mathcal{F}^{m_0}$ *if* $m_0 \in \operatorname{Int} C$ *and* $[g]_{P^X} \in \operatorname{Cl} \mathcal{F}^{m_0}_{P^X} \subseteq \mathcal{L}^2(P^X)$ *if* $P^X(\{\tilde{m}_0\}) = 0$*.*

(v) Let $Q_\ell := P_{n_{k_\ell}}$ *for each* ℓ*. If* $P^X(\{\tilde{m}_0\}) = 0$*, then* $\liminf_{\ell\to\infty} L(g_{k_\ell}, Q_\ell) \geq L(g, P) \geq L^*_{m_0}(P)$*.*

(vi) If $P_n = P$ *for all* n*, then we can ensure that the conclusions of (iii) and (iv) hold in all cases, even when the assumptions on* $\tilde{m}_0$ *are dropped.*

Proof. Fix a subsequence $(g_k)_{k=1}^\infty \equiv (f_{n_k})_{k=1}^\infty$. In the setting of Proposition 3.5.14, we have $m_{n_k} \to m_0$, so if $0 \leq z < m_0 < w \leq 1$, then all but finitely many of the functions g_k are convex on $[0, z]$ and concave on $[w, 1]$. Since $\{g_k(x)\}_{k=1}^\infty$ is bounded for all $x \in \operatorname{Int} C$ by Lemma 3.6.9, it follows from Rockafellar (1997, Theorem 10.9) and Lemma 3.6.12 that whenever $0 \leq z < m_0 < w \leq 1$, there is a subsequence of (g_k) that converges pointwise on $C \setminus (z, w)$. By considering sequences $z_n \nearrow m_0$ and $w_n \searrow m_0$ with $z_n < m_0 < w_n$ for all n, we deduce by a diagonal argument that (g_k) has a subsequence that converges pointwise to some $g\colon C \setminus \{\tilde{m}_0\} \to \mathbb{R}$ on $C \setminus \{\tilde{m}_0\}$ and uniformly on closed subsets of $C \setminus \{\tilde{m}_0\}$.

To extend g to $[0, 1] \setminus \{\tilde{m}_0\}$, we set $g(x) = g(M_L)$ for all $x \in [0, M_L)$ and $g(x) = g(M_R)$ for all $x \in (M_R, 1]$ if $m_0 \in \operatorname{Int} C$, and otherwise set $g(x) = 0$ for all $x \in [0, 1] \setminus C$ if $m_0 \notin \operatorname{Int} C$. Finally, by extracting a further subsequence (g_{k_ℓ}) if necessary, we can ensure that $g_{k_\ell}(\tilde{m}_0)$ converges to some $L \in [-\infty, \infty]$ as $\ell \to \infty$, and we extend g to $[0, 1]$ by setting $g(\tilde{m}_0) = L$.

(i) This follows from the construction of g in the first paragraph. Note also that if $m_0 \notin \operatorname{Int} C$, then g is increasing on C, and g is either concave or convex on C, depending on whether $\tilde{m}_0 = M_L$ or $\tilde{m}_0 = M_R$ respectively.

(ii) By the continuity of g on $C \setminus \{\tilde{m}_0\}$ and the uniform convergence established above, we deduce that if $z_\ell \to z \in C \setminus \{\tilde{m}_0\}$, then

$$|g_{k_\ell}(z_\ell) - g(z)| \leq |g_{k_\ell}(z_\ell) - g(z_\ell)| + |g(z_\ell) - g(z)| \to 0. \tag{3.6.36}$$

(iii) If $\tilde{m}_0 > M_L$, then $L = \lim_{\ell\to\infty} g_{k_\ell}(\tilde{m}_0) \geq \lim_{x\nearrow\tilde{m}_0} \lim_{\ell\to\infty} g_{k_\ell}(x) = \lim_{x\nearrow\tilde{m}_0} g(x)$, so $L \in (-\infty, \infty]$. Similarly if $\tilde{m}_0 < M_R$, then $L \leq \lim_{x\searrow\tilde{m}_0} g(x)$, whence $L \in [-\infty, \infty)$.

(iv) If $m_0 \in \operatorname{Int} C$, then $g \in \mathcal{F}^{m_0}$ by construction. Suppose now that $P^X(\{\tilde{m}_0\}) = 0$. Since $Q_\ell \xrightarrow{d} P$ under the hypotheses of Proposition 3.5.14, Skorokhod's representation theorem (e.g. van der Vaart, 1998, Theorem 2.19) guarantees the existence of random vectors $(X, Y), (X_1, Y_1), (X_2, Y_2), \ldots$ defined on a common probability space such that $(X, Y) \sim P$, $(X_\ell, Y_\ell) \sim Q_\ell$ for all ℓ and $(X_\ell, Y_\ell) \to (X, Y)$ almost surely. Then it follows from (3.6.36) that $g_{k_\ell}(X_\ell) \to g(X)$ almost surely on the event $\{X = \tilde{m}_0\}$, which has probability 1 since $P^X(\{\tilde{m}_0\}) = 0$ by assumption. An application of Fatou's lemma shows that

$$\begin{aligned}
\infty > \limsup_{n\to\infty} L(f_n, P_n) \geq \liminf_{\ell\to\infty} L(g_{k_\ell}, Q_\ell) &= \liminf_{\ell\to\infty} \mathbb{E}\big(\{Y_\ell - g_{k_\ell}(X_\ell)\}^2\big) \\
&\geq \mathbb{E}\Big(\liminf_{\ell\to\infty} \{Y_\ell - g_{k_\ell}(X_\ell)\}^2\Big) \\
&= \mathbb{E}\big(\{Y - g(X)\}^2\big) = L(g, P).
\end{aligned} \tag{3.6.37}$$

Thus, $\mathbb{E}\big(g(X)^2\big)^{1/2} \leq \mathbb{E}\big(\{Y - g(X)\}^2\big)^{1/2} + \mathbb{E}(Y^2)^{1/2} < \infty$, so $g \in L^2(P^X)$. By Proposition 3.5.12(d) and the proof of (i) above, it follows that $[g]_{P^X} \in \operatorname{Cl} \mathcal{F}^{m_0}_{P^X} \subseteq \mathcal{L}^2(P^X)$.

(v) Since $L(h_n, P) \to L(h, P)$ whenever $\|h_n - h\|_{L^2(P^X)} \to 0$, it follows from (3.6.37) and the conclusion of (iv) that $\liminf_{\ell\to\infty} L(g_{k_\ell}, Q_\ell) \geq L(g, P) \geq L^*_{m_0}(P)$, as required.

(vi) If $P_n = P$ for all n, then we can modify the argument leading up to (3.6.37) as follows: since $g_{k_\ell} \to g$ pointwise on C and $P^X(C) = 1$, it follows that if $(X, Y) \sim P$, then $g_{k_\ell}(X) \to g(X)$

(almost surely) and $\infty > \liminf_{\ell\to\infty} L(g_{k_\ell}, P) \geq L(g, P)$, as in (3.6.37). Thus, $g \in L^2(P^X)$ and $[g]_{P^X} \in \mathrm{Cl}\,\mathcal{F}^{m_0}_{P^X} \subseteq \mathcal{L}^2(P^X)$ as in the proof of (iv). In particular, when $\tilde{m}_0 \notin \mathrm{Int}\, C$ and $P^X(\{\tilde{m}_0\}) > 0$, we must have $g(\tilde{m}_0) \in \mathbb{R}$ since $g \in L^2(P^X)$. In this case, if $m_0 \in C$, then $g \sim_{P^X} h$ for some $h \in \mathcal{F}^{m_0}$, and otherwise if $m_0 \notin C$, then $[g]_{P^X} \in \mathrm{Cl}\,\mathcal{F}^{m_0}_{P^X}$ by Proposition 3.5.12(d). We conclude as before that $\liminf_{\ell\to\infty} L(g_{k_\ell}, P) \geq L(g, P) \geq L^*_{m_0}(P)$ in all cases, so the proof of Lemma 3.6.11 is complete. □

Proof of Proposition 3.5.14. (a) Fix $\varepsilon > 0$. By Proposition 3.5.12(a) and the observation in the paragraph after (3.5.38), there exists a continuous $h_0 \in \mathcal{F}^{m_0}$ such that $L^*_{m_0}(P) \leq L(h_0, P) \leq L^*_{m_0}(P) + \varepsilon$. Now for $\eta \in [-m_0, 1-m_0]$, define $h_\eta \colon [0,1] \to \mathbb{R}$ by $h_\eta(x) := h_0(0 \vee (x-\eta) \wedge 1)$. Then $h_\eta \in \mathcal{F}^{m_0+\eta}$ and $\sup_{x\in[0,1]} |h_\eta(x)| \leq |h_0(0)| \vee |h_0(1)| =: B$ for all $\eta \in [-m_0, 1-m_0]$. In addition, it follows from Lemma 3.6.13 that $h_\eta \to h_0$ uniformly on $[0,1]$ as $\eta \to 0$. For each n, let $\eta_n := m_n - m_0$, so that $h_{\eta_n} \in \mathcal{F}^{m_n}$ and

$$L^*_{m_n}(P_n) \leq L(h_{\eta_n}, P_n) = L(h_0, P_n) + \bigl(L(h_{\eta_n}, P_n) - L(h_0, P_n)\bigr)$$

by the definition of $L^*_{m_n}(P_n)$. Observe that

$$\begin{aligned}
|L(h_{\eta_n}, P_n) - L(h_0, P_n)| &\leq \int_{[0,1]\times\mathbb{R}} \Bigl|\bigl(y - h_{\eta_n}(x)\bigr)^2 - \bigl(y - h_0(x)\bigr)^2\Bigr| \, dP_n(x,y) \\
&\leq \int_{[0,1]\times\mathbb{R}} |h_0(x) - h_{\eta_n}(x)| \bigl(2|y| + |h_0(x)| + |h_{\eta_n}(x)|\bigr) \, dP_n(x,y) \\
&\leq \sup_{x\in[0,1]} |h_0(x) - h_{\eta_n}(x)| \int_{[0,1]\times\mathbb{R}} 2(|y| + B) \, dP_n(x,y).
\end{aligned}$$

Moreover, $W_2(P_n, P) \to 0$ by assumption, so $\int_{[0,1]\times\mathbb{R}} \|w\|^2 \, dP_n(w) \to \int_{[0,1]\times\mathbb{R}} \|w\|^2 \, dP(w)$. Thus, since $\bigl(y - h_0(x)\bigr)^2 \leq 2(y^2 + B^2)$ and $|y| \leq (1+y^2)/2$ for all $(x,y) \in [0,1]\times\mathbb{R}$, we deduce using Lemma 3.6.14 and the continuity of h_0 that

$$\begin{aligned}
L(h_0, P_n) = \int_{[0,1]\times\mathbb{R}} \bigl(y - h_0(x)\bigr)^2 \, dP_n(x,y) &\to \int_{[0,1]\times\mathbb{R}} \bigl(y - h_0(x)\bigr)^2 \, dP(x,y) = L(h_0, P) \\
\text{and} \quad \int_{[0,1]\times\mathbb{R}} (|y| + B) \, dP_n(x,y) &\to \int_{[0,1]\times\mathbb{R}} (|y| + B) \, dP(x,y) < \infty
\end{aligned}$$

as $n \to \infty$. Since $h_{\eta_n} \to h_0$ uniformly on $[0,1]$ as $n \to \infty$, it follows from the above that

$$\limsup_{n\to\infty} L^*_{m_n}(P_n) \leq \lim_{n\to\infty} L(h_0, P_n) = L(h_0, P) \leq L^*_{m_0}(P) + \varepsilon.$$

Since $\varepsilon > 0$ was arbitrary, this yields (a).

The proofs of (b)–(i) are based on the key Lemmas 3.6.9, 3.6.10 and 3.6.11 above.

(b) Fix a deterministic, non-negative sequence (δ_n) with $\delta_n \to 0$ and let (f_n) be any sequence with $f_n \in \psi^{\delta_n}_{m_n}(P_n)$ for all n, so that $L(f_n, P_n) \leq L^*_{m_n}(P_n) + \delta_n$ for all n. Then $\limsup_{n\to\infty} L(f_n, P_n) = \limsup_{n\to\infty} L^*_{m_n}(P_n) \leq L^*_{m_0}(P) < \infty$ by (a), so (f_n) satisfies the hypotheses of Lemma 3.6.11. In particular, Lemma 3.6.11(v) applies to every subsequence of (f_n) when $P^X(\{\tilde{m}_0\}) = 0$, in which case

$$\liminf_{n\to\infty} L^*_{m_n}(P_n) = \liminf_{n\to\infty} L(f_n, P_n) \geq L^*_{m_0}(P). \tag{3.6.38}$$

(c) If in addition $P_n = P$ for all n, then Lemma 3.6.11(vi) applies to every subsequence of (f_n), regardless of whether or not $P^X(\{\tilde{m}_0\}) = 0$, so (3.6.38) holds in all cases. Together with part (a) above, this establishes (c) and the fact that $L^*(P)$ and $\mathcal{I}^*(P)$ are well-defined.

(d) If $P^X(\{m\}) = 0$ for all $m \in [0,1]$, then (a) and (b) imply that for any sequence (m_n') in $[0,1]$ converging to some $m' \in [0,1]$, we have $\lim_{n\to\infty} L^*_{m_n'}(P_n) = L^*_{m'}(P)$. In other words, the functions $m \mapsto L^*_m(P_n)$ converge continuously to $m \mapsto L^*_m(P)$ on $[0,1]$ in the sense of Remmert (1991, Chapter 3.1.5). Since continuous convergence is equivalent to uniform convergence on the compact space $[0,1]$ (e.g. Remmert, 1991, pages 98–99), the first part of (d) follows. This in turn implies the second assertion that $L^*(P_n) = \min_{m\in[0,1]} L^*_m(P_n) \to \min_{m\in[0,1]} L^*_m(P) = L^*(P)$ as $n \to \infty$.

(e) Let (m_n') be any sequence in $[0,1]$ with $m_n' \in \mathcal{I}^{\delta_n}(P_n)$ for all n. For each subsequence of (m_n'), we may extract a further subsequence (m_{n_k}') that converges to some $m' \in [0,1]$. For each k, we have $L^*(P_{n_k}) \le L^*_{m_{n_k}'}(P_{n_k}) \le L^*(P_{n_k}) + \delta_{n_k}$ by the definition of $\mathcal{I}^{\delta_{n_k}}(P_{n_k})$. Thus, if $P^X(\{m\}) = 0$ for all $m \in [0,1]$, then for any $m^* \in \mathcal{I}^*(P)$, we deduce from (a) and (b) that

$$L^*(P) \le L^*_{m'}(P) = \lim_{k\to\infty} L^*_{m_{n_k}'}(P_{n_k}) = \lim_{k\to\infty} L^*(P_{n_k}) \le \lim_{k\to\infty} L^*_{m^*}(P_{n_k}) = L^*_{m^*}(P) = L^*(P),$$

so $m' \in \mathcal{I}^*(P)$ and $L^*(P_{n_k}) \to L^*(P)$ as $k \to \infty$. This shows that every subsequence of (m_n') has a further subsequence that converges to an element of $\mathcal{I}^*(P)$. Since (m_n') was arbitrary, this implies (e). Similarly, every subsequence of $\big(L^*(P_n)\big)$ has a further subsequence that converges to $L^*(P)$; this is another way to obtain the second part of (d).

For (f)–(i), fix any sequence (f_n) with $f_n \in \psi^{\delta_n}_{m_n}(P_n)$ for all n. If $P^X(\{\tilde{m}_0\}) = 0$, then for any subsequence $(g_k)_{k=1}^\infty \equiv (f_{n_k})_{k=1}^\infty$ of (f_n), we can find a further subsequence (g_{k_ℓ}) and a function g on $[0,1]$ satisfying conditions (i)–(v) in Lemma 3.6.11. In particular, setting $m_\ell' := m_{n_{k_\ell}}$ and $Q_\ell := P_{n_{k_\ell}}$, we deduce from (a) and Lemma 3.6.11(v) that

$$L(g,P) \le \liminf_{\ell\to\infty} L(g_{k_\ell}, Q_\ell) \le \limsup_{\ell\to\infty} L(g_{k_\ell}, Q_\ell) = \limsup_{\ell\to\infty} L^*_{m_\ell'}(Q_\ell) \le L^*_{m_0}(P),$$

where the equality above follows from the fact that $L(g_{k_\ell}, Q_\ell) \le L^*_{m_\ell'}(Q_\ell) + \delta_{m_{k_\ell}}$ for all ℓ. We conclude from Lemma 3.6.11(iv) and Corollary 3.5.13(c) that $g \in \psi^*_{\tilde{m}_0}(P) = \psi^*_{m_0}(P)$.

(f) For each closed set $A \subseteq (\operatorname{supp} P^X) \setminus \{\tilde{m}_0\}$, Lemma 3.6.11(ii) asserts that $g_{k_\ell} \to g \in \psi^*_{m_0}(P)$ uniformly on A. Thus, every subsequence of (f_n) has a further subsequence that converges uniformly on A to an element of $\psi^*_{m_0}(P)$, and by Corollary 3.5.13(a), all elements of $\psi^*_{m_0}(P)$ agree P^X-almost everywhere on A. Since (f_n) was arbitrary, (f) follows.

(g) If $\psi^0_{\tilde{m}_0}(P) \neq \emptyset$, then by Corollary 3.5.13(a), there exists $f^* \in \psi^0_{\tilde{m}_0}(P)$ such that $\psi^*_{\tilde{m}_0}(P) = [f^*]_{P^X}$, so $g \sim_{P^X} f^*$ in the argument before (f). Thus, in view of Lemma 3.6.11(i), we may assume that $g \in \mathcal{F}^{\tilde{m}_0}$, so that $g \in \psi^0_{\tilde{m}_0}(P)$. By applying Lemma 3.6.11(ii) as above, we deduce that for any closed set $A \subseteq (\operatorname{supp} P^X) \setminus \{\tilde{m}_0\}$, every subsequence of (f_n) has a further subsequence that converges uniformly on A to an element of $\psi^0_{\tilde{m}_0}(P)$. All functions in $\psi^0_{\tilde{m}_0}(P)$ agree on A by Corollary 3.5.13(e), and (f_n) was arbitrary, so (g) holds.

Suppose in addition that $m_0 \in \operatorname{Int}(\operatorname{csupp} P^X)$ and $P^X(\{m_0\}) = 0$. Then in the argument before (f), we can insist that $g \in \mathcal{F}^{m_0}$ in view of Lemma 3.6.11(iv), so that $g \in \psi^0_{m_0}(P)$.

(h) For fixed $q \in [1,\infty)$, Lemma 3.6.10 implies that there exists $\tilde{B} < \infty$ such that $|g_{k_\ell} - g|^q \le 2^{q-1}(\tilde{B}^q + |g|^q)$ on $[0,1]$ for all sufficiently large ℓ, so $\|g_{k_\ell} - g\|^q_{L^q(P^X)} = \int_{[0,1]} |g_{k_\ell} - g|^q \, dP^X \to 0$ by the dominated convergence theorem. In summary, every subsequence of $\big([f_n]_{P^X}\big)_{n=1}^\infty$ has a further subsequence that converges in $\mathcal{L}^q(P^X)$ to $\psi^*_{m_0}(P)$, so the entire sequence converges in $\mathcal{L}^q(P^X)$ to $\psi^*_{m_0}(P)$, as required.

(i) Under the hypotheses of (i), all elements of $\psi^0_{m_0}(P)$ are continuous by Corollary 3.5.13(f), so we can apply Lemmas 3.6.11(ii) and 3.6.13 to obtain the stronger conclusion that every subsequence of (f_n) has a further subsequence that converges uniformly on $\operatorname{csupp} P^X$ to some function in $\psi^0_{m_0}(P)$. Since elements of $\psi^0_{m_0}(P)$ agree on $\operatorname{supp} P^X$ by assumption and (f_n) was arbitrary, (i) holds. $\square$

Proof of Corollary 3.5.15. (a) By definition, we have $\psi^0(P) = \{f \in \mathcal{F} : L(f,P) = L^*(P)\} = \bigcup_{m\in\mathcal{I}^*(P)} \psi^0_m(P)$, and if $\psi^0_m(P) \neq \emptyset$ for some $m \in \mathcal{I}^*(P)\setminus \operatorname{csupp} P^X$, then $\tilde{m} = \operatorname{argmin}_{x\in\operatorname{csupp} P^X}|x-m|$ satisfies $\tilde{m} \in \mathcal{I}^*(P) \cap \operatorname{csupp} P^X$ and $\psi^0_{\tilde{m}}(P) \neq \emptyset$ by Corollary 3.5.13(c). The result now follows from Corollary 3.5.13(d).

For (b)–(d), fix a sequence (f_n) with $f_n \in \psi^{\delta_n}(P_n)$ for all n, so that there exists a sequence (m_n) in $[0,1]$ with $m_n \in \mathcal{I}^{\delta_n}(P_n)$ and $f_n \in \psi^{\delta_n}_{m_n}(P_n)$ for all n. By assumption, we have $P^X(\{m\}) = 0$ for all $m \in [0,1]$, so for each subsequence of (f_n), Proposition 3.5.14(e) ensures the existence of a further subsequence (f_{n_k}) such that $m_{n_k} \to m^*$ for some $m^* \in \mathcal{I}^*(P)$. Let $\tilde{m}^* := \operatorname{argmin}_{x\in\operatorname{csupp} P^X}|m^*-x|$. Then $L^*_{\tilde{m}^*}(P) = L^*_{m^*}(P) = L^*(P)$ by Corollary 3.5.13(c), so $\tilde{m}^* \in \mathcal{I}^*(P)$. We are now in a position to apply Proposition 3.5.14(f)–(i).

(b) Fix a closed set $A \subseteq (\operatorname{supp} P^X) \setminus \mathcal{I}^*(P) \subseteq (\operatorname{supp} P^X) \setminus \{\tilde{m}^*\}$. For any $f^* \in \psi^*_{m^*}(P) \subseteq \psi^*(P)$, Proposition 3.5.14(f) implies that $\|f_{n_k} - f^*\|_{L^\infty(A,P^X)} \to 0$. Thus, every subsequence of (f_n) has a further subsequence that converges in $\|\cdot\|_{L^\infty(A,P^X)}$ to an element of $\psi^*(P)$. Since (f_n) was arbitrary, this yields (b).

(c) Fix a closed set $A \subseteq (\operatorname{supp} P^X) \setminus \tilde{\mathcal{I}}^*(P)$.

- If $\tilde{m}^* \notin \tilde{\mathcal{I}}^*(P)$, then $\tilde{m}^* = m^* \in \operatorname{Int}(\operatorname{csupp} P^X)$ and all elements of $\psi^0_{\tilde{m}^*}(P) = \psi^0_{m^*}(P) \neq \emptyset$ are continuous, so for any $f^* \in \psi^0_{m^*}(P) \subseteq \psi^0(P)$, Proposition 3.5.14(i) implies that $f_{n_k} \to f^*$ uniformly on $\operatorname{supp} P^X \supseteq A$.
- If $\tilde{m}^* \in \tilde{\mathcal{I}}^*(P)$, then we still have $\tilde{m}^* \in \mathcal{I}^*(P) \cap \operatorname{csupp} P^X$, so $\psi^0_{\tilde{m}^*}(P) \neq \emptyset$ by assumption. Thus, for any $f^* \in \psi^0_{\tilde{m}^*}(P) \subseteq \psi^0(P)$, Proposition 3.5.14(g) implies that $f_{n_k} \to f^*$ uniformly on $(\operatorname{supp} P^X) \setminus \{\tilde{m}^*\} \supseteq A$.

Thus, every subsequence of (f_n) has a further subsequence that converges uniformly on A to an element of $\psi^0(P)$. Since (f_n) was arbitrary, (c) follows.

(d) Here, $m^* \in \mathcal{I}^*(P) \subseteq \operatorname{Int}(\operatorname{csupp} P^X)$ by assumption, so for any $f^* \in \psi^0_{m^*}(P) \subseteq \psi^*(P)$, Proposition 3.5.14(h) implies that $\|f_{n_k} - f^*\|_{L^q(P^X)} \to 0$ for any $q \in [1,\infty)$. By the same reasoning as in (b, c), we obtain (d). □

Proof of Proposition 3.5.16. In the definition of P_0, we have $\mathbb{E}(f_0(X) + \xi \,|\, X) = f_0(X)$ since ξ is independent of X and has mean 0 by (ii), so f_0 is a regression function for P_0 (in the sense of (3.5.38) in Section 3.1). It now follows from condition (iii) and Corollary 3.5.13(d) that $\psi^0_m(P_0) \neq \emptyset$ for all $m \in \operatorname{csupp} P_0^X$, so in particular $\psi^0(P_0) \neq \emptyset$.

Writing (D_n) for any one of the sequences of random variables in (a)–(d), we aim to prove that $D_n \xrightarrow{p} 0$, or equivalently that every subsequence (D_{n_k}) has a further subsequence that converges almost surely to 0. If it can be shown that $W_2(\mathbb{P}_n, P_0) \xrightarrow{p} 0$, then we can take $(D_{n_{k_\ell}})$ to be a subsequence of (D_{n_k}) such that $W_2(\mathbb{P}_{n_{k_\ell}}, P_0) \to 0$ almost surely. Working on an event Ω_0 of probability 1 on which this convergence takes place, we deduce directly from the relevant parts of Proposition 3.5.14 or Corollary 3.5.15 that $D_{n_{k_\ell}} \to 0$ on Ω_0; note that assertions (a, b) follow from Proposition 3.5.14(d, e) and assertions (c, d) follow from Corollary 3.5.15(c, d).

To complete the proof, we must therefore verify that $W_2(\mathbb{P}_n, P_0) \xrightarrow{p} 0$ under conditions (i)–(iii). It suffices to show that

$$(*)\ \mathbb{P}_n \xrightarrow{d} P_0 \text{ almost surely} \qquad \text{and} \qquad (**)\ \int_{\mathbb{R}^2} \|w\|^2\, d\mathbb{P}_n(w) \xrightarrow{p} \int_{\mathbb{R}^2} \|w\|^2\, dP_0(w),$$

since then we can argue along subsequences of $(\mathbb{P}_n)$ as in the previous paragraph.

$(*)$ Let $\tilde{\mathbb{P}}_n := n^{-1}\sum_{i=1}^n \delta_{(x_{ni},\xi_{ni})}$ for each n and define $\tilde{P}_0 := P_0^X \otimes P_\xi$. Defining the map $F_0\colon (x,z) \mapsto (x, f_0(x) + z)$ on $\mathbb{R}^2$, we therefore have $\mathbb{P}_n = \tilde{\mathbb{P}}_n \circ F_0^{-1}$ for each n and $P_0 = \tilde{P}_0 \circ F_0^{-1}$. The desired convergence statement $(*)$ follows from the following two claims.

Claim. *$\tilde{\mathbb{P}}_n \xrightarrow{d} \tilde{P}_0$ almost surely.*

Proof of Claim. By Billingsley (1999, Theorem 2.3), $\mathcal{R} := \{[a_1, b_1] \times [a_2, b_2] : a_j \leq b_j$ and $a_j, b_j \in \mathbb{Q}$ for $j = 1, 2\}$ is a countable convergence-determining class in the sense of Billingsley (1999, page 18), so it suffices to show that $\tilde{\mathbb{P}}_n(R) \to \tilde{P}_0(R)$ almost surely for each $R \in \mathcal{R}$. To this end, fix any $I_1 \times I_2 \in \mathcal{R}$, where $I_j = [a_j, b_j]$ is an interval with rational endpoints $a_j \leq b_j$ for $j = 1, 2$. By condition (i), $\mathbb{P}_n^X \xrightarrow{d} P_0^X$ and $P_0^X(\{a_1, b_1\}) = 0$, so $\mathbb{P}_n^X(I_1) \to P_0^X(I_1)$ as $n \to \infty$. For each n, defining $r_n := \sum_{i=1}^n \mathbb{1}_{\{x_{ni} \in I_1\}} = n\mathbb{P}_n^X(I_1)$, we can write $\tilde{\mathbb{P}}_n(I_1 \times I_2) = \mathbb{P}_n^X(I_1)\, T_n$, where

$$T_n := \frac{\sum_{i=1}^n \mathbb{1}_{\{x_{ni} \in I_1\}} \mathbb{1}_{\{\xi_{ni} \in I_2\}}}{r_n \vee 1} \sim \frac{1}{r_n \vee 1} \operatorname{Bin}\bigl(r_n, P_\xi(I_2)\bigr).$$

If $P_0^X(I_1) = 0$, then certainly $\tilde{\mathbb{P}}_n(I_1 \times I_2) = \mathbb{P}_n^X(I_1)\, T_n \to 0 = P_0^X(I_1)P_\xi(I_2) = \tilde{P}_0(I_1 \times I_2)$. On the other hand, if $P_0^X(I_1) > 0$, then $r_n = n\bigl(1 + o(1)\bigr)P_0^X(I_1) \to \infty$, so for all $t > 0$, we have $\sum_{n=1}^\infty \mathbb{P}(|T_n - P_\xi(I_2)| > t) < \infty$ by Hoeffding's inequality (or some other suitable exponential tail bound for binomial random variables; see van der Vaart and Wellner (1996, Appendix A.6.1) for example). Thus, by the first Borel–Cantelli lemma, $T_n \to P_\xi(I_2)$ almost surely, so $\tilde{\mathbb{P}}_n(I_1 \times I_2) = \mathbb{P}_n^X(I_1)\, T_n \to P_0^X(I_1)P_\xi(I_2) = \tilde{P}_0(I_1 \times I_2)$ almost surely as $n \to \infty$, as required. □

Claim. *If (Q_n) is any sequence of probability measures such that $Q_n \xrightarrow{d} \tilde{P}_0$, then $Q_n \circ F_0^{-1} \xrightarrow{d} \tilde{P}_0 \circ F_0^{-1} = P_0$ under condition (iii).*

Proof of Claim. By Skorokhod's representation theorem (e.g. van der Vaart, 1998, Theorem 2.19), there exist random vectors $(\tilde{X}, \tilde{Z}), (\tilde{X}_1, \tilde{Z}_1), (\tilde{X}_2, \tilde{Z}_2), \dots$ defined on a common probability space such that $(\tilde{X}, \tilde{Z}) \sim \tilde{P}_0$, $(\tilde{X}_n, \tilde{Z}_n) \sim Q_n$ for all n and $(\tilde{X}_n, \tilde{Z}_n) \to (\tilde{X}, \tilde{Z})$ almost surely.

Since $\tilde{X} \sim P_0^X$ and f_0 is continuous P_0^X-almost everywhere under condition (iii), we have $f_0(\tilde{X}_n) \to f_0(\tilde{X})$ almost surely, so $F_0(\tilde{X}_n, \tilde{Z}_n) = (\tilde{X}_n, f_0(\tilde{X}_n) + \tilde{Z}_n) \to (\tilde{X}, f_0(\tilde{X}) + \tilde{Z}) = F_0(\tilde{X}, \tilde{Z})$ almost surely. Thus, the distribution $Q_n \circ F_0^{-1}$ of $F_0(\tilde{X}_n, \tilde{Z}_n)$ converges weakly to the distribution $\tilde{P}_0 \circ F_0^{-1} = P_0$ of $F_0(\tilde{X}, \tilde{Z})$, as required. □

$(**)$ Let $X \sim P_0^X$ and $\xi \sim P_\xi$ be independent, so that $\bigl(X, f_0(X) + \xi\bigr) \sim P_0$. We have

$$\int_{\mathbb{R}^2} \|w\|^2 \, d\mathbb{P}_n(w) = \frac{1}{n}\sum_{i=1}^n (x_{ni}^2 + Y_{ni}^2) = \frac{1}{n}\sum_{i=1}^n \bigl(x_{ni}^2 + f_0^2(x_{ni}) + 2f_0(x_{ni})\,\xi_{ni} + \xi_{ni}^2\bigr) \tag{3.6.39}$$

and now consider each of the summands on the right-hand side. Since $(\mathbb{P}_n^X)$ is a sequence of probability measures on the compact set $[0, 1]$ satisfying $\mathbb{P}_n^X \xrightarrow{d} P_0^X$, we have $W_2(\mathbb{P}_n^X, P_0^X) \to 0$, so

$$\frac{1}{n}\sum_{i=1}^n x_{ni}^2 = \int_{[0,1]} x^2 \, d\mathbb{P}_n^X(x) \to \int_{[0,1]} x^2 \, dP_0^X(x) = \mathbb{E}(X^2). \tag{3.6.40}$$

In addition, we can apply condition (iii) and argue as in the proof of the first Claim to see that $\mathbb{P}_n^X \circ f_0^{-1} \xrightarrow{d} P_0^X \circ f_0^{-1}$. Since f_0 is bounded on $[0, 1]$ by (iii), these probability measures are also supported on some compact set, so in fact $W_2\bigl(\mathbb{P}_n^X \circ f_0^{-1}, P_0^X \circ f_0^{-1}\bigr) \to 0$, whence

$$\frac{1}{n}\sum_{i=1}^n f_0^2(x_{ni}) = \int_{\mathbb{R}} x^2 \, d\bigl(\mathbb{P}_n^X \circ f_0^{-1}\bigr)(x) = \int_{\mathbb{R}} x^2 \, d\bigl(\mathbb{P}_0^X \circ f_0^{-1}\bigr)(x) = \mathbb{E}\bigl(f_0^2(X)\bigr). \tag{3.6.41}$$

For all $t > 0$, it follows from (3.6.41), condition (ii) and Chebsyhev's inequality that

$$\mathbb{P}\biggl(\frac{1}{n}\biggl|\sum_{i=1}^n f_0(x_{ni})\,\xi_{ni}\biggr| > t\biggr) \leq \frac{1}{(nt)^2}\operatorname{Var}\biggl(\sum_{i=1}^n f_0(x_{ni})\,\xi_{ni}\biggr) = \frac{1}{(nt)^2}\sum_{i=1}^n f_0^2(x_{ni})\operatorname{Var}(\xi) \to 0, \tag{3.6.42}$$

so $n^{-1}\sum_{i=1}^n f_0(x_{ni})\,\xi_{ni} \xrightarrow{p} 0 = \mathbb{E}\bigl(f_0(X)\xi\bigr)$ by the independence of X and ξ. Finally, by condition (ii), $\xi_{n1},\ldots,\xi_{nn} \overset{\mathrm{iid}}{\sim} P_\xi$ for each n, so $n^{-1}\sum_{i=1}^n \xi_{ni}^2 \xrightarrow{p} \mathbb{E}(\xi^2)$ by the weak law of large numbers. Together with (3.6.39), (3.6.40), (3.6.41) and (3.6.42), this implies that

$$\int_{\mathbb{R}^2} \|w\|^2\,d\mathbb{P}_n(w) \xrightarrow{p} \mathbb{E}(X^2) + \mathbb{E}\bigl(f_0^2(X)\bigr) + 2\mathbb{E}\bigl(f_0(X)\xi\bigr) + \mathbb{E}(\xi^2) = \int_{\mathbb{R}^2} \|w\|^2\,dP_0(w),$$

so $(**)$ holds. $\square$

Proof of Proposition 3.1.2. The results for $(\tilde{g}_n) = (\tilde{f}_n)$ follow immediately from Proposition 3.5.16. When $(\tilde{g}_n) = (\hat{f}_n^{m_0})$, we again have $W_2(\mathbb{P}_n, P_0) \xrightarrow{p} 0$ under conditions (i)–(iii) in Proposition 3.5.16, so assertions (a, b, c, d) follow from Proposition 3.5.14(e, g, i, h) in this case. $\square$

3.6.4 Auxiliary results and examples for Section 3.5.4

The proofs in Section 3.6.3 make use of two straightforward results on the convergence of sequences of S-shaped functions.

Lemma 3.6.12. *Suppose that $(f_n)_{n=1}^\infty$ is a sequence of increasing convex functions on $[0,1)$ such that $\lim_{n\to\infty} f_n(x)$ exists for all $x \in (0,1)$. Then $\lim_{n\to\infty} f_n(0)$ exists and the function $f\colon [0,1) \to \mathbb{R}$ defined by $f(x) := \lim_{n\to\infty} f_n(x)$ is convex and increasing. Moreover, $f_n \to f$ uniformly on $[0,w]$ for every $w \in [0,1)$.*

Proof. Since $f_n|_{(0,1)}$ is convex and increasing for all n, the same is true of the pointwise limit $f|_{(0,1)}$. Thus, $l := \lim_{t\searrow 0} f(t)$ exists and is finite, and we now show that $f_n(0) \to l$ as $n \to \infty$. Since each f_n is convex on $[0,1)$, we have $f_n(0) \geq 2f_n(t) - f_n(2t)$ for all $t > 0$ and $n \in \mathbb{N}$, so

$$\liminf_{n\to\infty} f_n(0) \geq \lim_{t\searrow 0}\,\lim_{n\to\infty} \bigl(2f_n(t) - f_n(2t)\bigr) = \lim_{t\searrow 0} \bigl(2f(t) - f(2t)\bigr) = l.$$

On the other hand, f_n is increasing on $[0,1)$ for all n, so

$$\limsup_{n\to\infty} f_n(0) \leq \lim_{t\searrow 0}\,\lim_{n\to\infty} f_n(t) = \lim_{t\searrow 0} f(t) = l,$$

which means that $f(0) = l$, as required. Consequently, f is convex and increasing on $[0,1)$. For the final assertion of the lemma, we extend $f, f_1, f_2, \ldots$ to increasing convex functions on $(-\infty,1)$ by setting $f(x) = f(0)$ and $f_n(x) = f_n(0)$ for all $x < 0$ and $n \in \mathbb{N}$. It follows from what we have already shown that $f_n \to f$ pointwise on $(-\infty,1)$, so in fact $f_n \to f$ uniformly on compact subsets of $(-\infty,1)$ by Rockafellar (1997, Theorem 10.8). This yields the desired conclusion. $\square$

Lemma 3.6.13. *If $m \in (0,1)$ and $(f_n)_{n=1}^\infty$ is a sequence of functions in $\mathcal{F}^m$ that converges pointwise on $[0,1] \setminus \{m\}$ to some continuous $f \in \mathcal{F}^m$, then $f_n \to f$ uniformly on $[0,1]$.*

Proof. First note that $f_n \to f$ pointwise on $[0,1]$. Indeed,

$$f(z) = \lim_{n\to\infty} f_n(z) \leq \liminf_{n\to\infty} f_n(m) \leq \limsup_{n\to\infty} f_n(m) \leq \lim_{n\to\infty} f_n(w) = f(w)$$

whenever $z < m < w$, and since $\lim_{z\nearrow m} f(z) = f(m) = \lim_{w\searrow m} f(w)$ by continuity, it follows that $f_n(m) \to f(m)$. We now show that $f_n \to f$ uniformly on $[0,1]$ by a standard argument: fix $\varepsilon > 0$ and note that since f is continuous and increasing on $[0,1]$, we can find $0 = z_0 < z_1 < \ldots < z_{k-1} < z_k = 1$ such that $f(z_i) - f(z_{i-1}) < \varepsilon$ for all $i \in [k]$. Since each f_n is increasing, we see that if $x \in [z_{i-1}, z_i]$, then

$$f_n(z_{i-1}) - f(z_{i-1}) - \varepsilon < f_n(z_{i-1}) - f(z_i) \leq f_n(x) - f(x) \leq f_n(z_i) - f(z_{i-1}) < f_n(z_i) - f(z_i) + \varepsilon.$$

Since $f_n \to f$ pointwise, $\limsup_{n\to\infty} \sup_{x\in[0,1]} |f_n(x) - f(x)| < \lim_{n\to\infty} \max_{1\leq i\leq k} |f_n(z_i) - f(z_i)| + \varepsilon = \varepsilon$. This holds for all $\varepsilon > 0$, so the result follows. $\square$

The weak convergence result below is stated as Lemma 4.5 in Dümbgen et al. (2011) and proved here for completeness.

Lemma 3.6.14. *Let $P, P_1, P_2, \dots$ be probability measures on $\mathbb{R}^d$ such that $P_n \xrightarrow{d} P$. If h is a non-negative, continuous function on $\mathbb{R}^d$ such that $\int_{\mathbb{R}^d} h\,dP_n \to \int_{\mathbb{R}^d} h\,dP < \infty$, then $\int_{\mathbb{R}^d} f\,dP_n \to \int_{\mathbb{R}^d} f\,dP$ for any continuous function $f\colon \mathbb{R}^d \to \mathbb{R}^k$ such that $\|f\|/(1+h)$ is bounded.*

Proof. We can restrict attention to the case $k = 1$ since the component functions can be considered separately when $k > 1$. Let $C > 0$ be such that $|f| \leq C(1+h)$ pointwise. For a Borel measure Q on $\mathbb{R}^d$ and a Q-integrable function h, we write $Q(h)$ as shorthand for $\int_{\mathbb{R}^d} h\,dQ$.

Since $P_n \xrightarrow{d} P$, we have $\liminf_{n\to\infty} P_n(g) \geq P(g)$ for all non-negative, continuous $g\colon \mathbb{R}^d \to \mathbb{R}$ by the portmanteau lemma (e.g. van der Vaart, 1998, Lemma 2.2(iv)). Thus, since $f^+ := f \vee 0$ and $C(1+h) - f^+$ are non-negative and continuous, we have $\liminf_{n\to\infty} P_n(f^+) \geq P(f^+)$ and $\liminf_{n\to\infty} P_n\bigl(C(1+h) - f^+\bigr) \geq P\bigl(C(1+h) - f^+\bigr)$. Moreover, $P_n\bigl(C(1+h)\bigr) \to P\bigl(C(1+h)\bigr)$ by assumption, so in fact $P_n(f^+) \to P(f^+)$. A similar argument shows that $P_n(f^-) \to P(f^-)$, where $f^- := (-f) \vee 0$, so we indeed have $P_n(f) \to P(f)$. $\square$

We conclude this subsection with a series of related examples which illustrate that some of the assertions of Proposition 3.5.14 and Corollary 3.5.15 do not hold in general if the associated technical conditions are not satisfied.

Example 3.2. First, we consider situations where either $P^X(\{\tilde{m}_0\}) > 0$ or $m_0 \notin \mathrm{Int}(\mathrm{csupp}\, P^X)$. In each of the following, we construct $P \in \mathcal{P}$ and a sequence (P_n) in $\mathcal{P}$ with $W_2(P_n, P) \to 0$, where $P = (1-\eta)Q + \eta\tilde{Q}$ and $P_n = (1-\eta_n)Q_n + \eta_n\tilde{Q}_n$ for suitable $Q, Q_n, \tilde{Q}_n \in \mathcal{P}$ and $\eta, \eta_n \in [0,1]$. For $w \in \mathbb{R}^d$ with $d \in \mathbb{N}$, we write δ_w for a point mass at w.

(a) Fix $m_0 \in (0,1]$ and $m \in (0, m_0]$. Let $Q_n := \frac{1}{2}\delta_{(0,0)} + \frac{1}{2}\delta_{(m(1-1/n),\,0)}$, $Q := \frac{1}{2}\delta_{(0,0)} + \frac{1}{2}\delta_{(m,0)}$, $\tilde{Q}_n = \tilde{Q} := \delta_{(m,1)}$ and $\eta_n = \eta := 1/3$ for all n. Then $P_n = \frac{1}{3}\delta_{(0,0)} + \frac{1}{3}\delta_{(m(1-1/n),\,0)} + \frac{1}{3}\delta_{(m,1)} \xrightarrow{d} \frac{1}{3}\delta_{(0,0)} + \frac{1}{3}\delta_{(m,0)} + \frac{1}{3}\delta_{(m,1)} = P$ and $P^X = \frac{1}{3}\delta_0 + \frac{2}{3}\delta_m$, so $m_0 \notin \mathrm{Int}(\mathrm{csupp}\, P^X)$, $\mathcal{I}^*(P) = [0,1] \not\subseteq \mathrm{Int}(\mathrm{csupp}\, P^X)$, $\tilde{m}_0 = m$ and $P^X(\{\tilde{m}_0\}) > 0$. Since $P, P_1, P_2, \dots$ are supported on the compact set $[0,1]^2$, we automatically have $W_2(P_n, P) \to 0$.

We claim that Propositions 3.5.14(b, d, h) and Corollary 3.5.15(d) do not apply here. Indeed, for each n, we have $f_n(m) = 1$ for all $f_n \in \psi^0_{m_0}(P_n) = \psi^0(P_n)$ and $L^*(P_n) = L^*_{m_0}(P_n) = 0$, whereas $f^*(m) = 1/2$ for all $f^* \in \psi^*_{m_0}(P) = \psi^*(P)$ and $L^*(P) = L^*_{m_0}(P) = 1/6 > 0 = \lim_{n\to\infty} L^*_{m_0}(P_n)$. Thus, if $f_n \in \psi^0_{m_0}(P_n)$ for all n, then $|f_n(m) - f^*(m)| = 1/2$ for all n and $f^* \in \psi^*(P)$, so $\inf_{f^*\in\psi^*(P)} \|f_n - f^*\|_{L^q(P^X)} \not\to 0$ for $q \in [1,\infty)$.

(b) This is a variant of (a) with $m = m_0 \in \mathrm{Int}(\mathrm{csupp}\, P^X) = (0,1)$ but $P^X(\{m_0\}) > 0$. Let Q_n, Q and η_n, η be as in (a) but instead define $\tilde{Q}_n = \tilde{Q} := \frac{1}{2}\delta_{(m_0,1)} + \frac{1}{2}\delta_{(1,1)}$. Then $P^X = \frac{1}{3}\delta_0 + \frac{1}{3}\delta_{m_0} + \frac{1}{3}\delta_1$ and all the deductions in the second paragraph of (a) remain valid here.

(c) Fix $m_0 \in (0,1]$ and $m \in (0, m_0]$. For $n \in \mathbb{N}$, let Q, Q_n be the uniform distributions on $\{(x,0) : 0 \leq x \leq m\}$ and $\{(x,0) : 0 \leq x \leq m(1-1/n)\}$ respectively. Moreover, let $\tilde{Q} := Q$, $\eta := 0$, $\tilde{Q}_n := \delta_{(m,n^2)}$ and $\eta_n := n^{-5}$ for all n. Then $P_n = (1-\eta_n)Q_n + \eta_n\tilde{Q}_n$ converges in W_2 to $P = Q$. Indeed, for any continuous $f\colon \mathbb{R}^2 \to \mathbb{R}$ such that $|f(x,y)| \leq 1 + x^2 + y^2$ for all $(x,y) \in \mathbb{R}^2$, we have $\eta_n f(m, n^2) = O(1/n)$, so $\int_{\mathbb{R}^2} f\,dP_n = (1-\eta_n)\int_0^{m(1-1/n)} f(x,0)\,dx + \eta_n f(m,n^2) \to \int_0^m f(x,0)\,dx = \int_{\mathbb{R}^2} f\,dP$ as $n \to \infty$.

Here, $\tilde{m}_0 = m$ and $P^X(\{m'\}) = 0$ for all $m' \in [0,1]$, but $m_0 \notin \mathrm{Int}(\mathrm{csupp}\, P^X)$, $\mathcal{I}^*(P) = [0,1] \not\subseteq \mathrm{Int}(\mathrm{csupp}\, P^X)$, and Proposition 3.5.14(h) and Corollary 3.5.15(d) do not hold. Indeed, for each n, let $f_n \in \psi^0_{m_0}(P_n) = \psi^0(P_n)$ be such that $f_n = 0$ on $[0, m(1-1/n)]$, $f_n(m) = n^2$ and f_n is linear on $[m(1-1/n), 1]$. Since $f^* = 0$ P^X-almost everywhere on $[0,m]$ for all $f^* \in \psi^*_{m_0}(P) = \psi^*(P)$, we have $\inf_{f^* \in \psi^*(P)} \|f_n - f^*\|_{L^q(P^X)} = \inf_{f^* \in \psi^*(P)} \|f_n\|_{L^q(P^X)} \geq \inf_{f^* \in \psi^*(P)} \|f_n\|_{L^1(P^X)} = n \to \infty$ for all $q \in [1,\infty)$.

In Proposition 3.5.14(i), the assumption that $\psi^0_{m_0}(P) \neq \emptyset$ and all elements of $\psi^0_{m_0}(P)$ agree on $\mathrm{supp}\, P^X$ is clearly necessary for the conclusion to hold (not least when $P_n = P$ for all n). When this condition is not satisfied, some elements of $\psi^0_{m_0}(P)$ are discontinuous by Corollary 3.5.13(e). If in addition $m_0 \in \mathrm{Int}(\mathrm{csupp}\, P^X) \cap \mathrm{supp}\, P^X$ and $P^X(\{m_0\}) = 0$, then Proposition 3.5.14(i) fails. This is demonstrated by the next example, which is a modification of Example 3.2(b).

Example 3.3. Fix $m \in (0,1)$ and for $n \in \mathbb{N}$, let $f_n \colon [0,1] \to [0,1]$ be such that $f_n = 0$ on $[0, m(1-1/n)]$, $f_n = 1$ on $[m,1]$, and f_n is continuous and linear on $[m(1-1/n), m]$. For each n, let P_n be the distribution supported on $\{(x, f_n(x)) : x \in [0,1]\}$ for which the corresponding marginal distribution P_n^X is the uniform distribution on $D := [0,m] \cup [m',1]$ for some $m' \in [m,1)$. Then (P_n) converges in W_2 to the uniform distribution P on $\{(x, \mathbb{1}_{[m,1]}(x)) : x \in D\}$.

Not all elements of $\psi^0(P) = \psi^0_m(P)$ agree at $m \in \mathrm{supp}\, P^X$; for example when $m' = m$ and $D = [0,1]$, the functions in $\psi^0_m(P)$ agree with $\mathbb{1}_{[m,1]}$ on $[0,1] \setminus \{m\}$ but can take any value in $[0,1]$ at m. We have $P^X(\{m\}) = 0$ and $m \in \mathrm{Int}(\mathrm{csupp}\, P^X)$, so the other conditions of Proposition 3.5.14(i) are satisfied, but $\psi^0(P_n) = \psi^0_m(P_n) = \{f_n\}$ for all n and (f_n) does not have a uniform limit on $[0,m] \subseteq \mathrm{supp}\, P^X$.

In Example 3.3, note in addition that while all the conditions of Corollary 3.5.15(c) are met, the associated convergence statement cannot be extended to $A = \mathrm{supp}\, P^X$. In general, Proposition 3.5.14(g) also does not hold with $A = \mathrm{supp}\, P^X$ under the stated conditions $P^X(\{\tilde{m}_0\}) = 0$ and $\psi^0_{\tilde{m}_0}(P) \neq \emptyset$.

To see this, we can instead take $D = [0,m]$ in Example 3.3 and fix $m_0 \in (m,1]$, so that $\tilde{m}_0 = m$, $P^X(\{\tilde{m}_0\}) = 0$ and $0 \in \psi^0_{\tilde{m}_0}(P)$. Then there is a sequence (g_n) with $g_n \in \psi^0_{m_0}(P_n)$ for all n but no uniform limit on $\mathrm{supp}\, P^X = [0,m]$; for example, let g_n be such that $g_n = 0$ on $[0, m(1-1/n)]$, $g_n(m) = 1$ and g_n is linear on $[m(1-1/n), 1]$.

Finally, we explain why $\mathcal{I}^*(P)$ is not always an interval (when P does not have an S-shaped regression function f_P), and that when $\psi^0(P)$ is non-empty, its elements need not agree on $\mathrm{supp}\, P^X$.

Example 3.4. For $P \in \mathcal{P}$ such that the corresponding marginal P^X has support $[0,1]$, it can be shown that the following hold:

(a) Suppose that P has a regression function $f_P \in \mathcal{F}^{m_0}$ for some m_0 and let $[a,b]$ be the largest subinterval containing m_0 on which f_P is linear. Then $m \mapsto L^*_m(P)$ is non-increasing on $[0,m_0]$ and non-decreasing on $[m_0,1]$, and attains its minimum value $L^*(P) = 0$ on $[a,b] \subseteq \mathcal{I}^*(P)$.

(b) Suppose that P has a regression function f_P that is non-decreasing on $[0,1]$, concave on $[0,m_0]$ and convex on $[m_0,1]$ for some $m_0 \in [0,1]$ (i.e. f_P is a 'back-to-front S-shaped function' with an inflection point at m_0). Then $m \mapsto L^*_m(P)$ is non-decreasing on $[0,m']$ and non-increasing on $[m',1]$ for some $m' \in [0,1]$, so $\mathcal{I}^*(P)$ contains either 0 or 1.

In (b), if in addition P^X is invariant under the map $x \mapsto 1-x$ and there is some $c \in \mathbb{R}$ such that $f_P(x) = c - f_P(1-x)$ for all $x \in [0,1]$, then $L^*_m(P) = L^*_{1-m}(P)$ for all $m \in [0,1]$, and $g \in \psi^0_m(P)$ if and only if $x \mapsto c - g(1-x)$ lies in $\psi^0_{1-m}(P)$. Thus, $\{0,1\} \subseteq \mathcal{I}^*(P)$, and except in some special cases, we generally have $1/2 \notin \mathcal{I}^*(P)$, in which case $\mathcal{I}^*(P)$ is not an interval, and the elements of $\psi^0(P)$ do not all agree on $\mathrm{supp}\, P^X$.

For example, suppose that $f_P(x) = (x - 1/2)^3$ for all $x \in [0, 1]$ and P^X is the uniform distribution on $[0, 1]$. Then the strict concavity and convexity of f_P on $[0, 1/2]$ and $[1/2, 1]$ respectively ensure that $\mathcal{I}^*(P) = \{0, 1\}$, and that $\psi^0(P)$ consists of a convex function f^* and a corresponding concave function $x \mapsto -f^*(1 - x)$, which do not agree on $\operatorname{supp} P^X$. If instead P^X is the uniform distribution on $D := \{i/n : 0 \leq i \leq n\}$ for some $n \in \mathbb{N}$ and f_P is as above, then $\mathcal{I}^*(P) = [0, 1/n] \cup [1 - 1/n, 1]$ due to the discreteness of P^X. Similarly, there is a convex function $f^* \in \psi^0(P)$ such that every $f^* \in \psi^0(P)$ agrees on D with either f^* or the corresponding concave function $x \mapsto -f^*(1 - x)$.

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